



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 114158

TO: Zohreh Fay
Location: Rem 4a59 / 4c70
Thursday, February 12, 2004
Art Unit: 1614
Phone: 272-0573
Serial Number: 09 / 551159

From: Jan Delaval
Location: Biotech-Chem Library
Rem 1A51
Phone: 272-2504

jan.delaval@uspto.gov

Search Notes

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Zohreh Fay Examiner #: 66646 Date: 2/11/04
 Art Unit: 1614 Phone Number 301-571272 Serial Number: 04551159
 Mail Box and Bldg/Room Location: 4C70 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Beta-Beta-Dihydroxy Meso-substituted chlorins, isobacteriochlorins and bacteriochlorins
 Inventors (please provide full names): _____

Macalpine, Jill ; Bruckner, Christian ; Dolphin, David

Earliest Priority Filing Date: 4/14/1999

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

please search the claimed compounds.

STAFF USE ONLY

Searcher: Jan
 Searcher Phone #: 22504
 Searcher Location: _____
 Date Searcher Picked Up: 2/12
 Date Completed: 2/12
 Searcher Prep & Review Time: _____
 Clerical Prep Time: 15
 Online Time: 40

Type of Search

NA Sequence (#) _____
 AA Sequence (#) _____
 Structure (#) ✓
 Bibliographic _____
 Litigation _____
 Fulltext _____
 Patent Family _____
 Other _____

Vendors and cost where applicable

STN ✓
 Dialog _____
 Questel/Orbit _____
 Dr.Link _____
 Lexis/Nexis _____
 Sequence Systems _____
 WWW/Internet _____
 Other (specify) _____

=> fil reg

FILE 'REGISTRY' ENTERED AT 18:58:04 ON 12 FEB 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 FEB 2004 HIGHEST RN 649538-27-2

DICTIONARY FILE UPDATES: 11 FEB 2004 HIGHEST RN 649538-27-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide can tot 149

L49 ANSWER 1 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 301530-03-0 REGISTRY

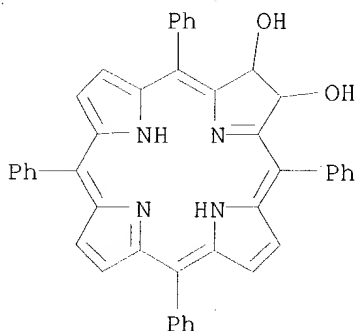
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MF C44 H31 N5 O4

CI IDS

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



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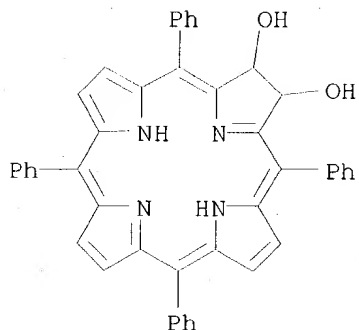
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L49 ANSWER 2 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 301530-02-9 REGISTRY

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MF C44 H32 N4 O3
CI IDS
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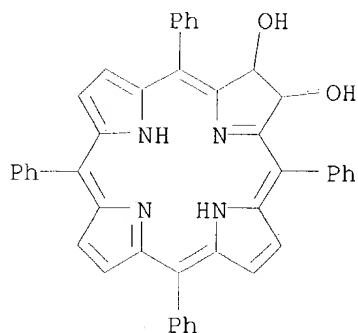


D1-OH

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CI IDS
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



D1-Br

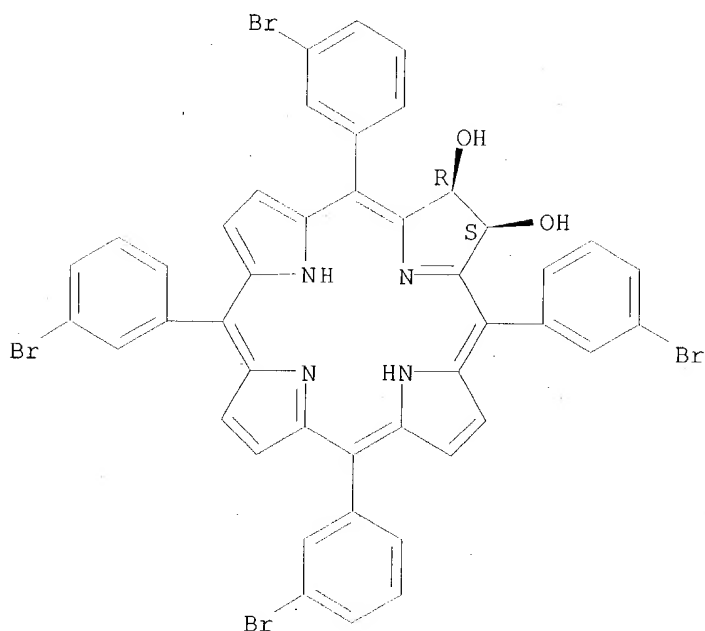
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RN 301338-12-5 REGISTRY
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, (7R,8S)-rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C44 H28 Br4 N4 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.



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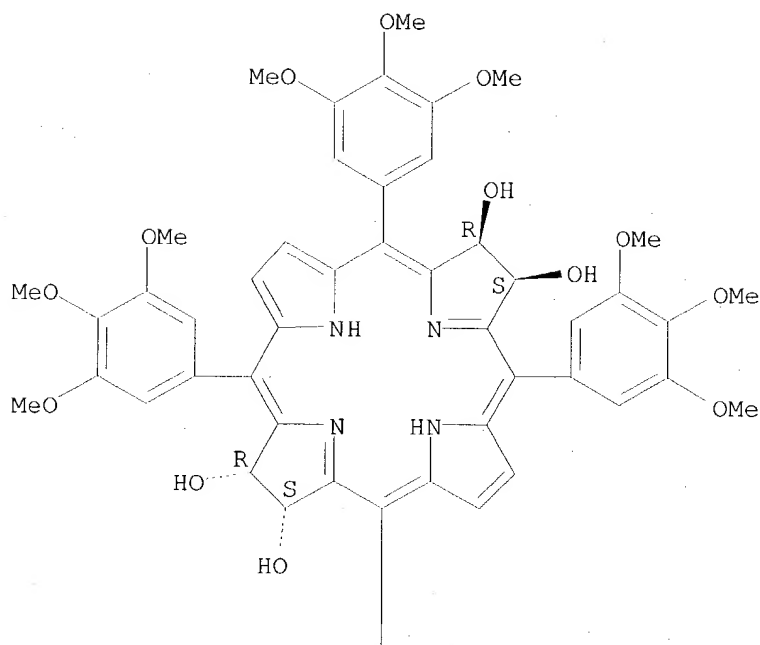
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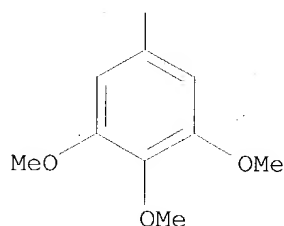
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RN 301337-23-5 REGISTRY
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FS STEREOSEARCH
MF C56 H58 N4 O16
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Relative stereochemistry.

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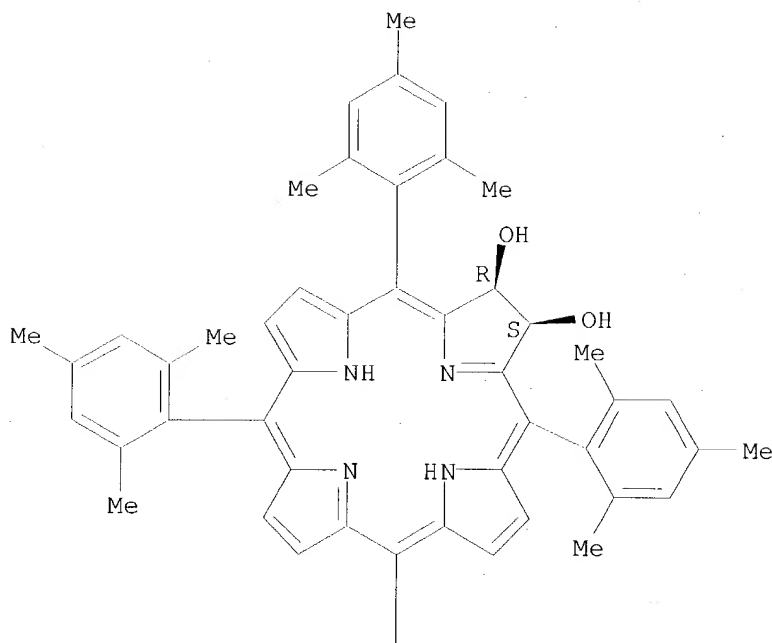
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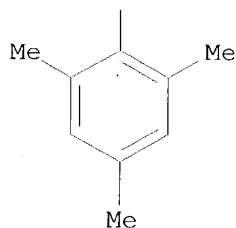
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RN **301337-13-3** REGISTRY
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FS STEREOSEARCH
MF **C56 H56 N4 O2**
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 7 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 301337-10-0 REGISTRY

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methylphenyl)-
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FS STEREOSEARCH

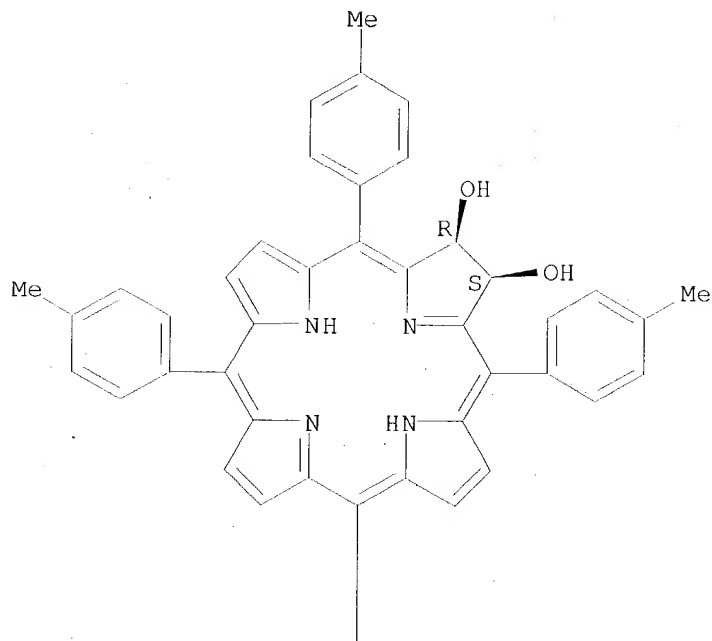
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SR CA

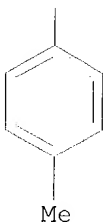
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

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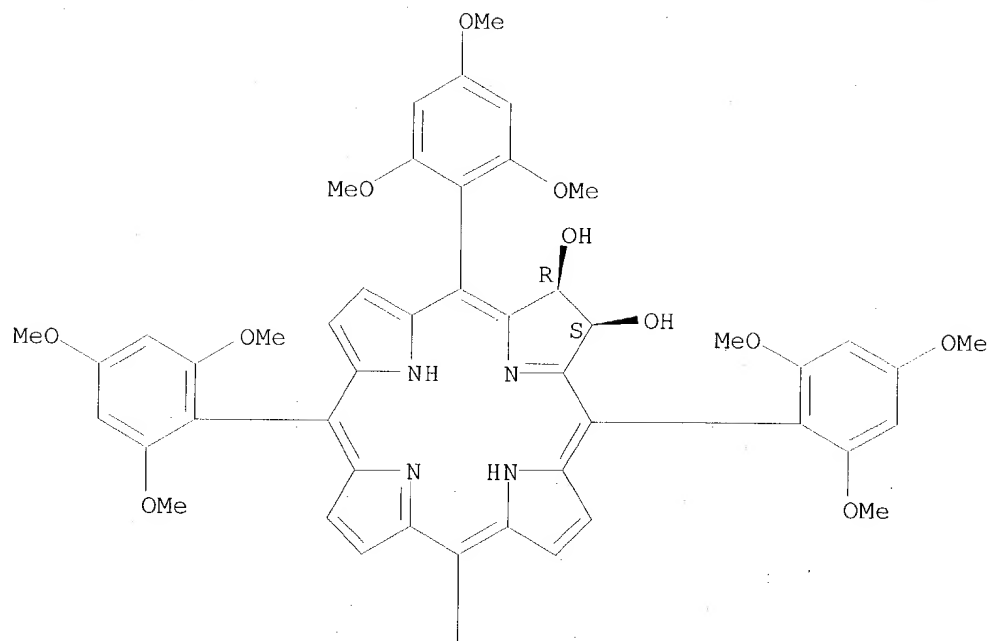
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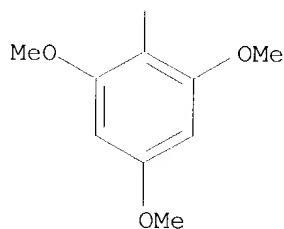
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RN 301337-07-5 REGISTRY
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FS STEREOSEARCH
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SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Relative stereochemistry.

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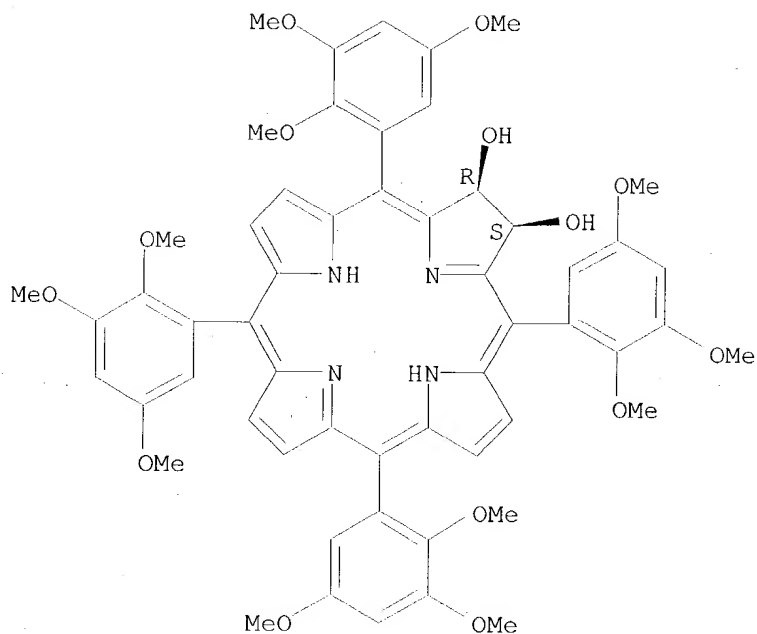
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L49 ANSWER 9 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN
RN 301337-05-3 REGISTRY
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,3,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C56 H56 N4 O14
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Relative stereochemistry.



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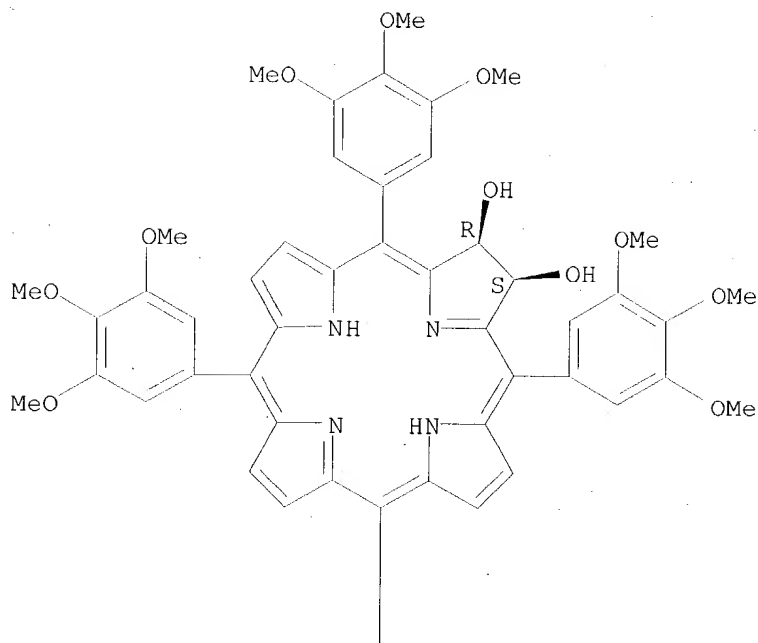
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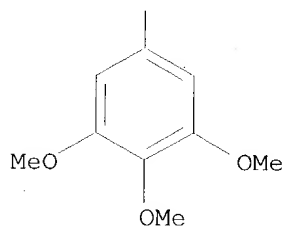
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RN 301337-03-1 REGISTRY
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FS STEREOSEARCH
MF C56 H56 N4 O14
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

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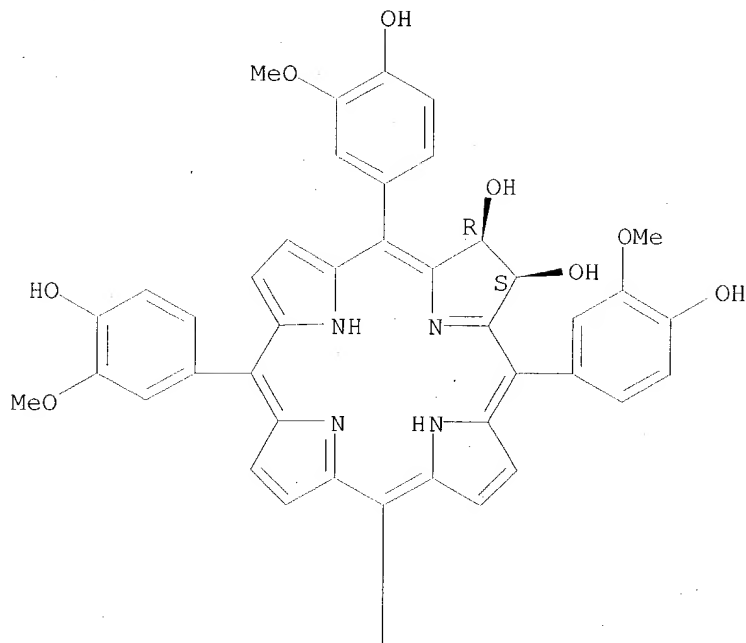
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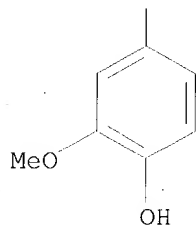
L49 ANSWER 11 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN
RN 301337-00-8 REGISTRY
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxy-3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C48 H40 N4 O10
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 12 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 301336-97-0 REGISTRY

CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3,5-dimethoxyphenyl)-
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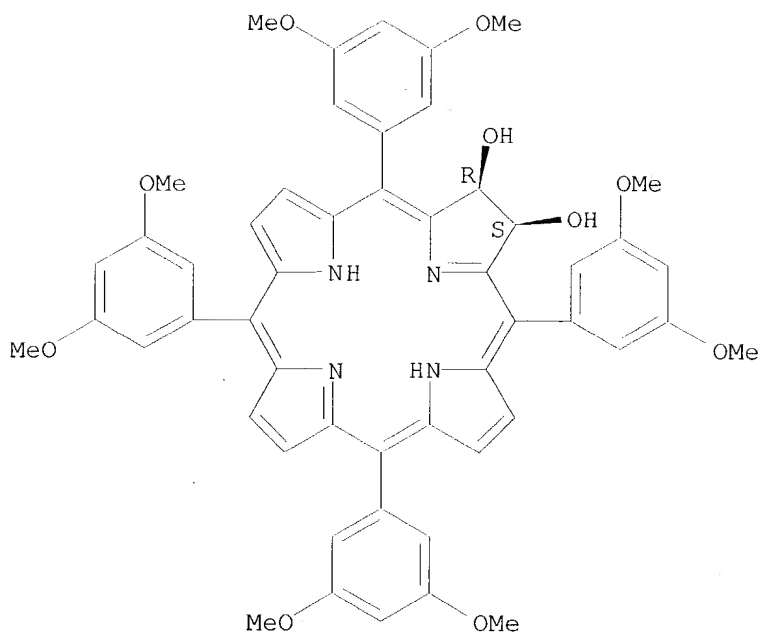
FS STEREOSEARCH

MF C52 H48 N4 O10

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 13 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 301336-94-7 REGISTRY

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

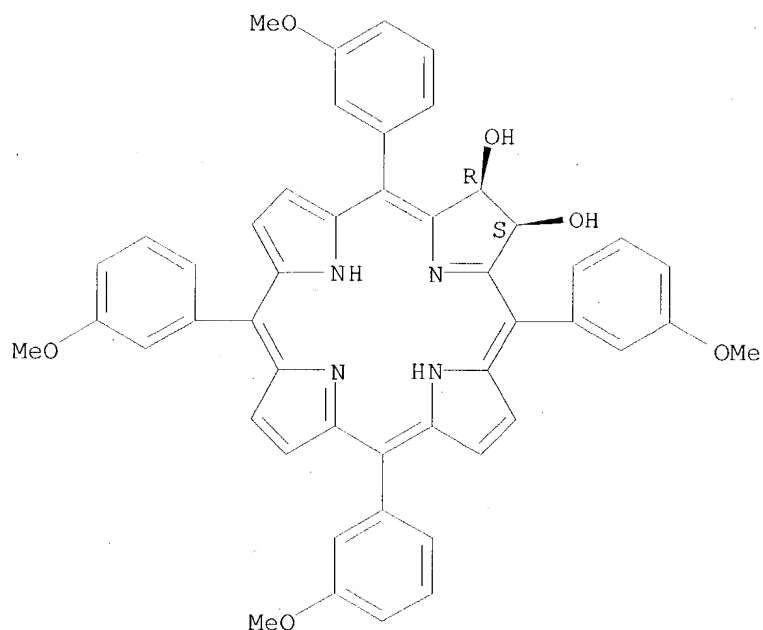
FS STEREOSEARCH

MF C48 H40 N4 O6

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.



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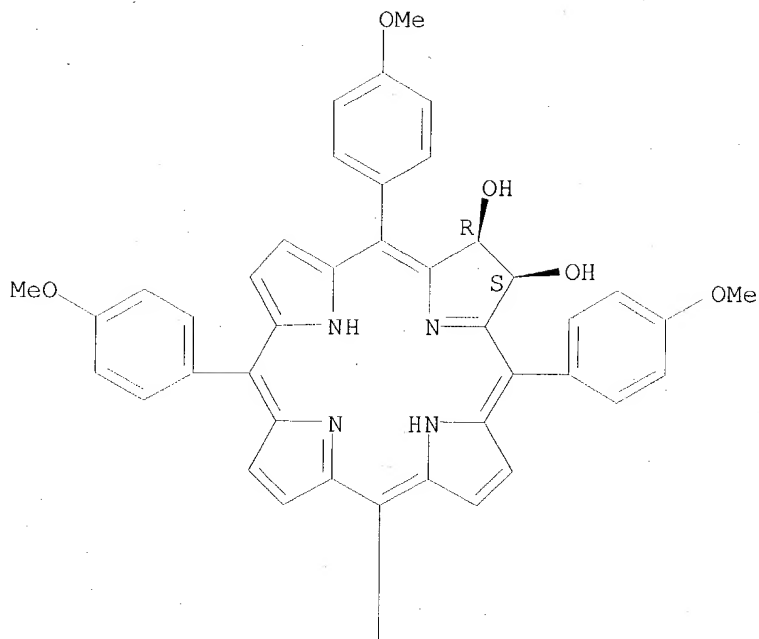
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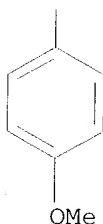
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RN 301336-91-4 REGISTRY
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FS STEREOSEARCH
MF C48 H40 N4 O6
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 15 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN **301336-88-9** REGISTRY

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis[4-(1-oxopropoxy)phenyl]-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

DR 478415-85-9

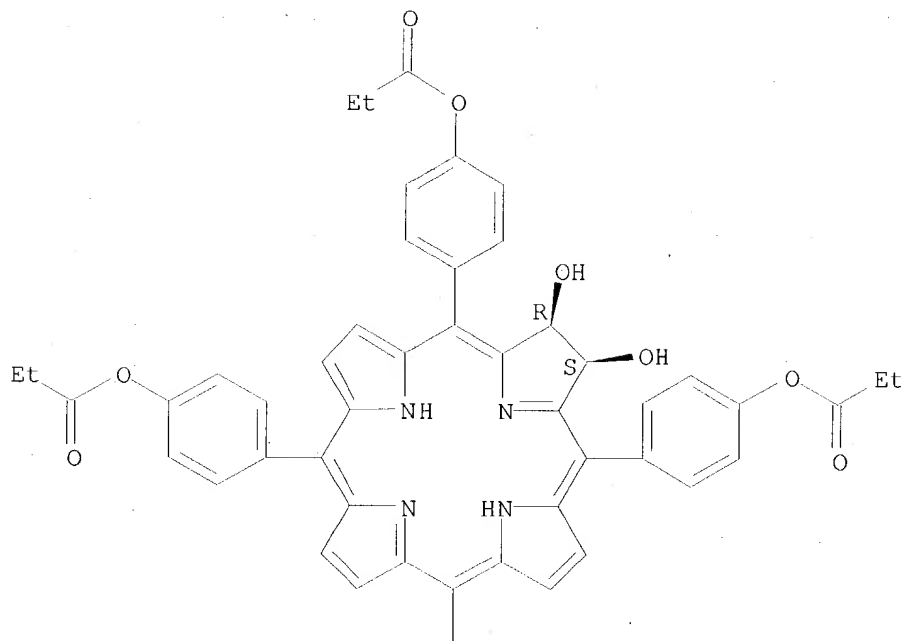
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SR CA

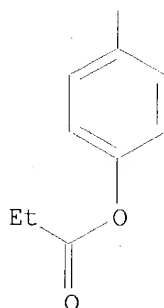
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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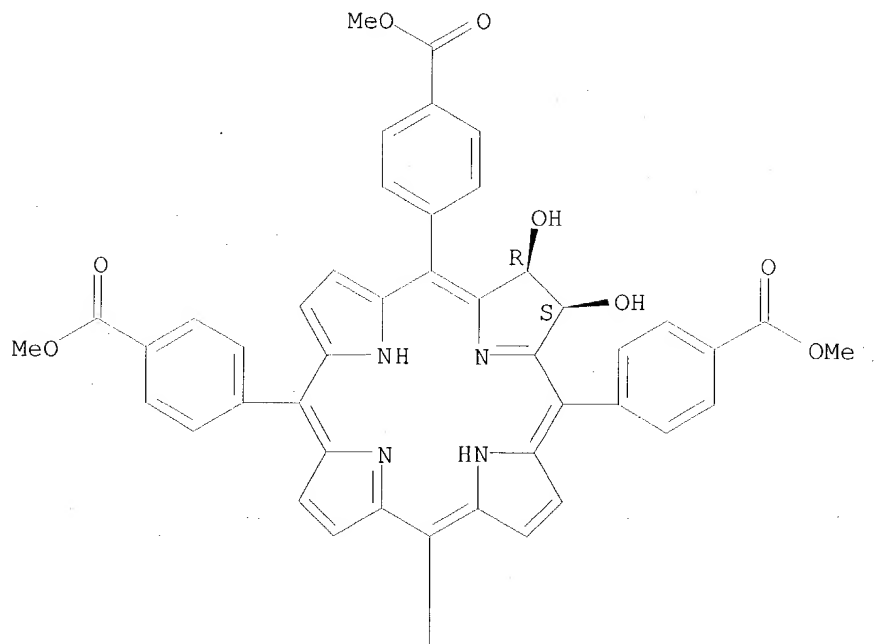
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L49 ANSWER 16 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN
RN 301336-85-6 REGISTRY
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FS STEREOSEARCH
MF C52 H40 N4 O10
SR CA

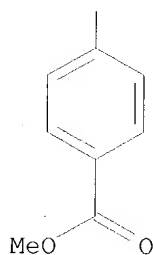
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Relative stereochemistry.

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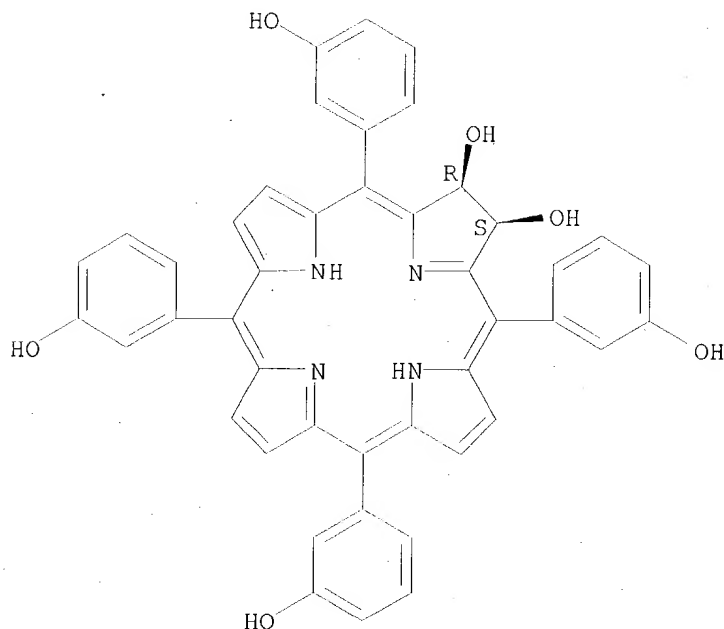
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L49 ANSWER 17 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN
RN 301336-82-3 REGISTRY
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FS STEREOSEARCH
MF C44 H32 N4 O6
SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
Relative stereochemistry.



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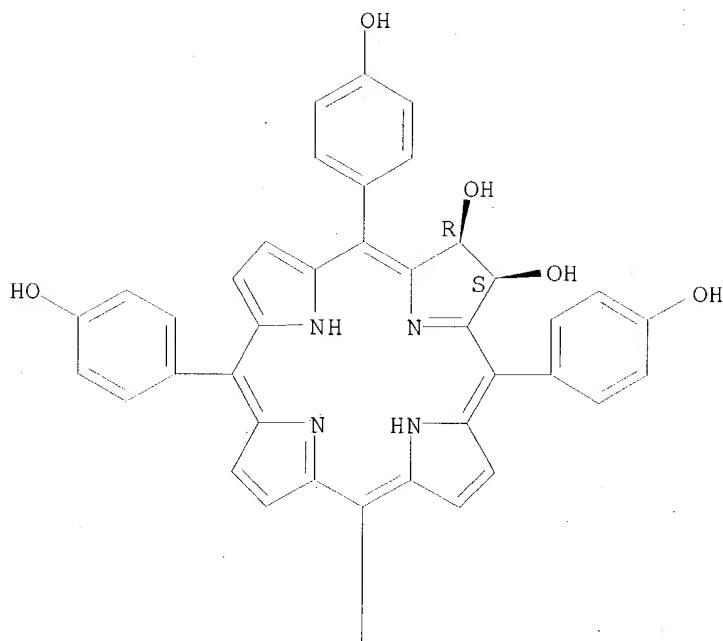
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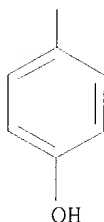
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RN 301336-78-7 REGISTRY
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FS STEREOSEARCH
MF C44 H32 N4 O6
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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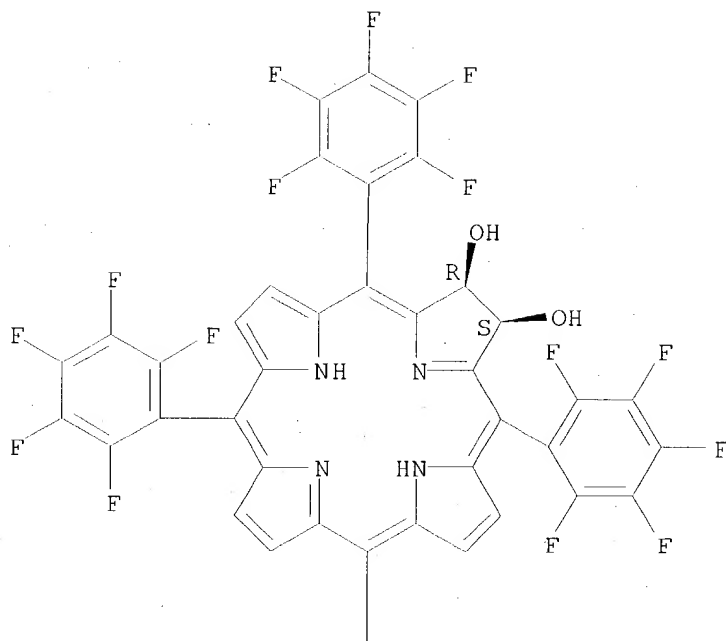
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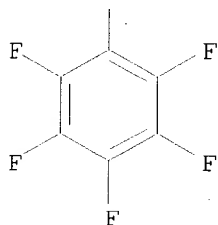
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RN **301336-74-3** REGISTRY
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tetraakis(pentafluorophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C44 H12 F20 N4 O2**
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 20 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN **301336-70-9** REGISTRY

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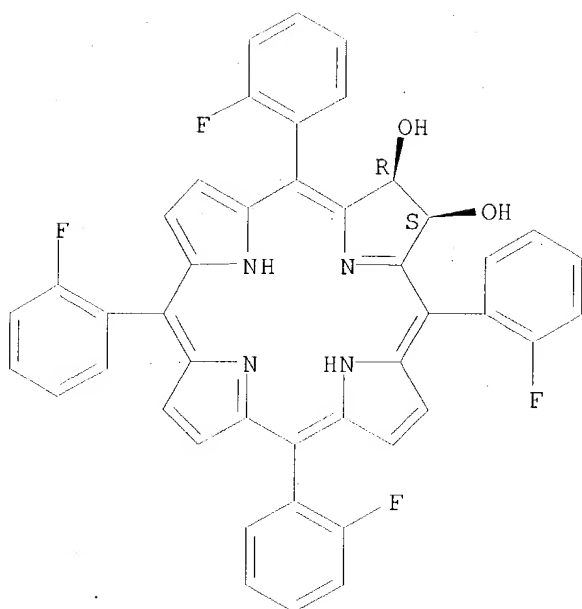
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SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 21 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN **301336-66-3** REGISTRY

CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3-fluorophenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

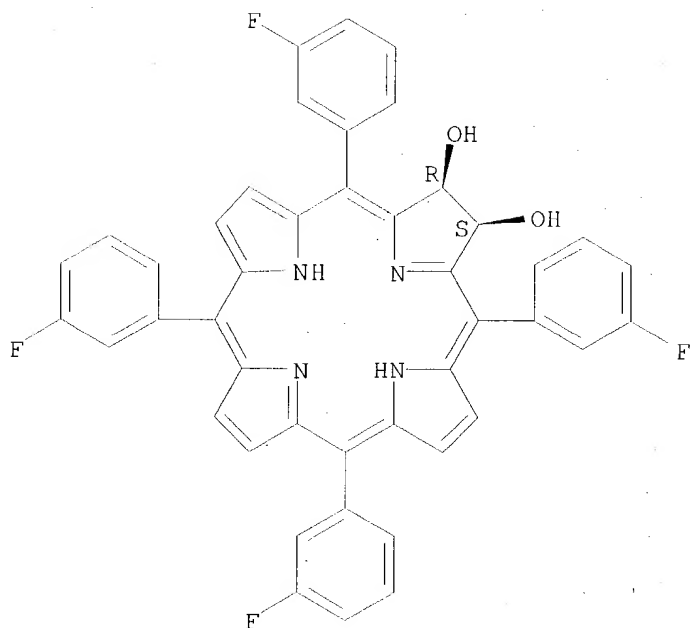
FS STEREOSEARCH

MF **C44 H28 F4 N4 O2**

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 22 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 301336-61-8 REGISTRY

CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(4-bromophenyl)-7,8-dihydro-
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

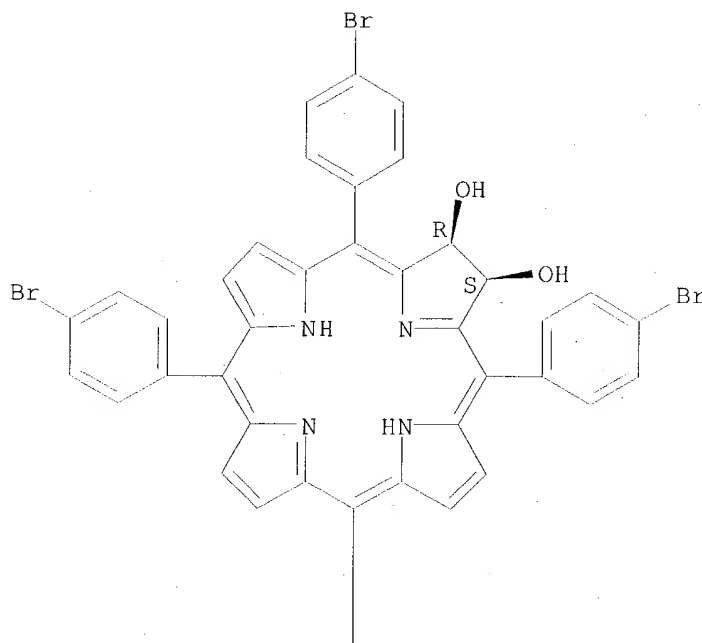
MF C44 H28 Br4 N4 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

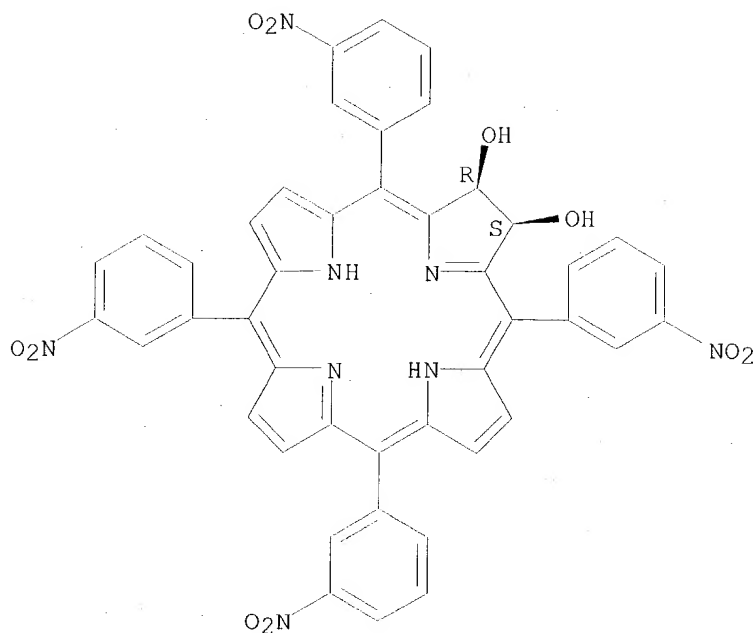
2 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 23. OF 26 REGISTRY COPYRIGHT 2004 ACS on STN
RN 301336-58-3 REGISTRY
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-nitrophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)
FS. STEREOSEARCH
MF C44 H28 N8 O10
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:39122

REFERENCE 2: 133:296322

L49 ANSWER 24 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 172925-98-3 REGISTRY

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7 α ,8 α ,17 β ,18 β)-

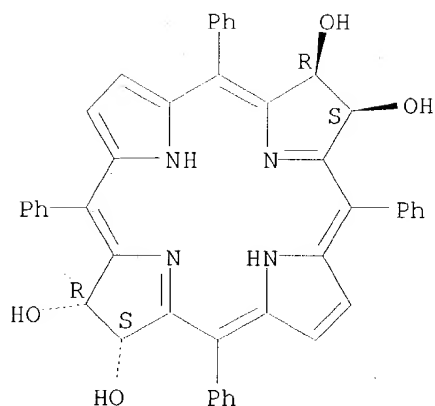
FS STEREOSEARCH

MF C44 H34 N4 O4

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:86084
REFERENCE 2: 133:296322
REFERENCE 3: 125:58205
REFERENCE 4: 124:116935

L49 ANSWER 25 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 172805-94-6 REGISTRY

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17R,18S)-rel- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

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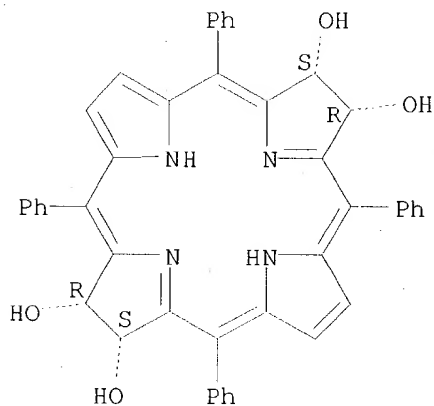
FS STEREOSEARCH

MF C44 H34 N4 O4

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:86084

REFERENCE 2: 125:58205

REFERENCE 3: 124:116935

L49 ANSWER 26 OF 26 REGISTRY COPYRIGHT 2004 ACS on STN

RN 165336-21-0 REGISTRY

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(CA INDEX NAME)

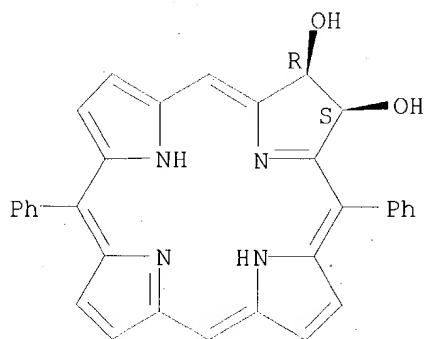
FS STEREOSEARCH

MF C32 H24 N4 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:39122

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REFERENCE 4: 133:296322

REFERENCE 5: 123:83046

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L49

26 S L46,L48

SAV L49 FAY551/A

FILE 'HCAOLD' ENTERED AT 18:57:10 ON 12 FEB 2004

L50

0 S L49

FILE 'HCAPLUS' ENTERED AT 18:57:14 ON 12 FEB 2004

L51 9 S L49
L52 5 S L51 AND L1-L3
L53 5 S L12,L52
L54 4 S L51 NOT L53
L55 9 S L51-L54

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L56 3 S L49

FILE 'REGISTRY' ENTERED AT 18:58:04 ON 12 FEB 2004

=> fil uspatall

FILE 'USPATFULL' ENTERED AT 18:58:26 ON 12 FEB 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 18:58:26 ON 12 FEB 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d l56 bib abs hitstr tot

L56 ANSWER 1 OF 3 USPATFULL on STN

AN 2003:246957 USPATFULL

TI 1,3-Dipolar cycloadditions to polypyrrolic macrocycles

IN MacAlpine, Jill Kirsten, Alexandria, VA, United States

Sternberg, Ethan D., Vancouver, CANADA

Dolphin, David, Vancouver, CANADA

PA University of British Columbia, British Columbia, CANADA (non-U.S. corporation)

PI US 6620929 B1 20030916

AI US 2000-551160 20000414 (9)

PRAI US 1999-129324P 19990414 (60)

DT Utility

FS GRANTED

EXNAM Primary Examiner: Berch, Mark L.; Assistant Examiner: Habte, Kahsay

LREP Morrison & Foerster LLP

CLMN Number of Claims: 15

ECL Exemplary Claim: 1

DRWN 8 Drawing Figure(s); 6 Drawing Page(s)

LN.CNT 1116

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Methods of modifying polypyrrolic macrocycles by use of a 1,3-dipolar cycloaddition are described. The methods may be used to produce compounds for further derivatization to produce photosensitizing agents of interest.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 165336-21-0P 172925-98-3P 301336-58-3P

301336-61-8P 301336-66-3P 301336-70-9P

301336-74-3P 301336-78-7P 301336-82-3P

301336-85-6P 301336-88-9P 301336-91-4P

301336-94-7P 301336-97-0P 301337-00-8P

301337-03-1P 301337-05-3P 301337-07-5P

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301338-12-5P 301530-01-8P 301530-02-9P

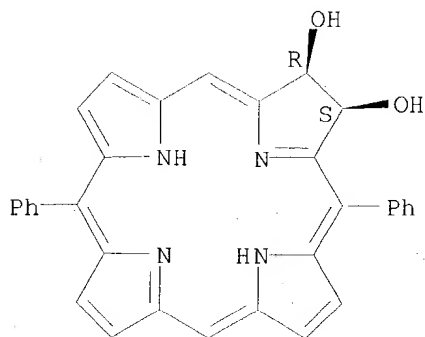
301530-03-0P

(synthesis of β,β , -dihydroxymeso-substituted chlorins, isobacteriochlorins, and bacteriochlorins with improved photosensitizer activity)

RN 165336-21-0 USPATFULL

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-diphenyl-, (7R,8S)-rel- (9CI)
(CA INDEX NAME)

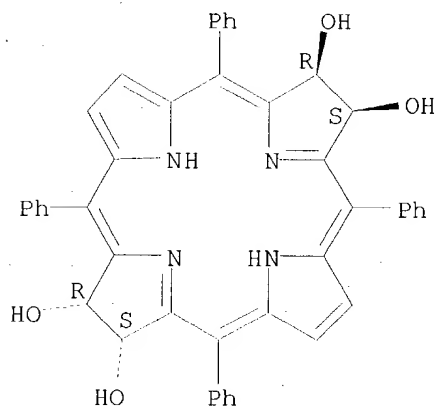
Relative stereochemistry.



RN 172925-98-3 USPATFULL

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

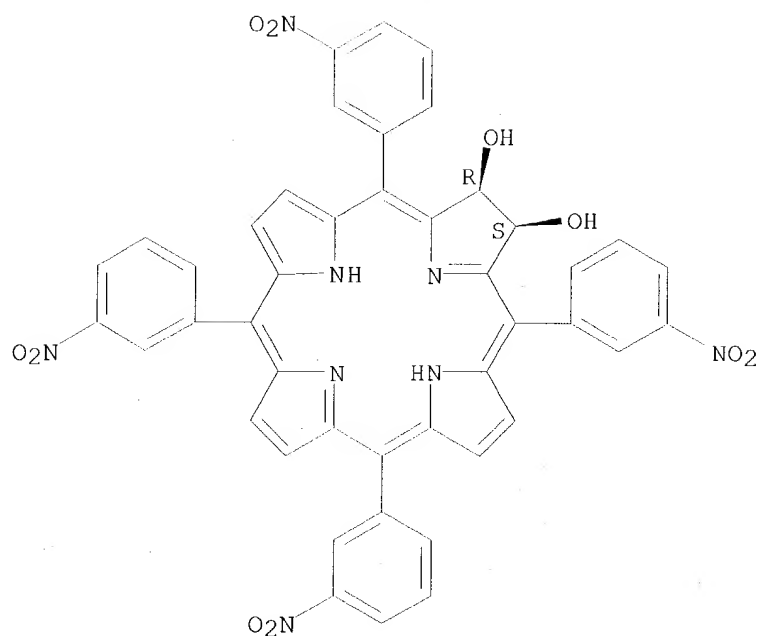
Relative stereochemistry.



RN 301336-58-3 USPATFULL

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-nitrophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

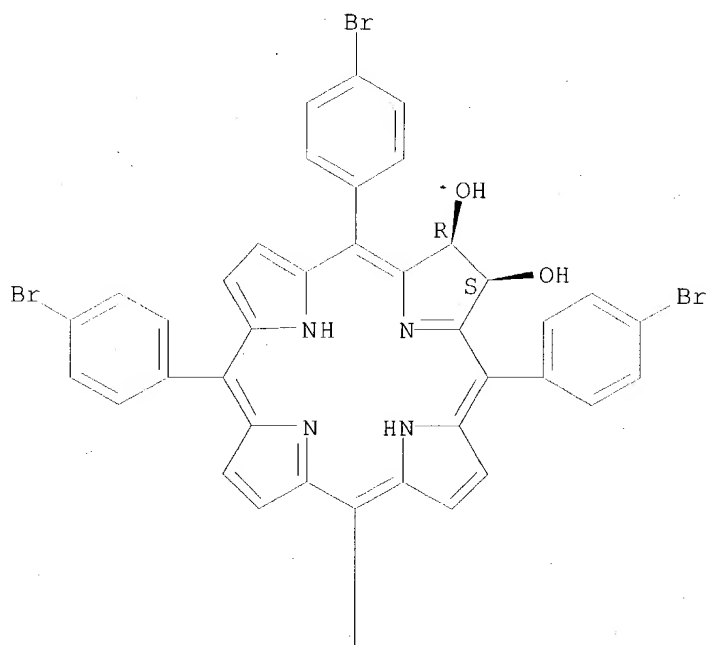
Relative stereochemistry.



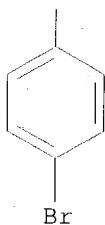
RN 301336-61-8 USPATFULL
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(4-bromophenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

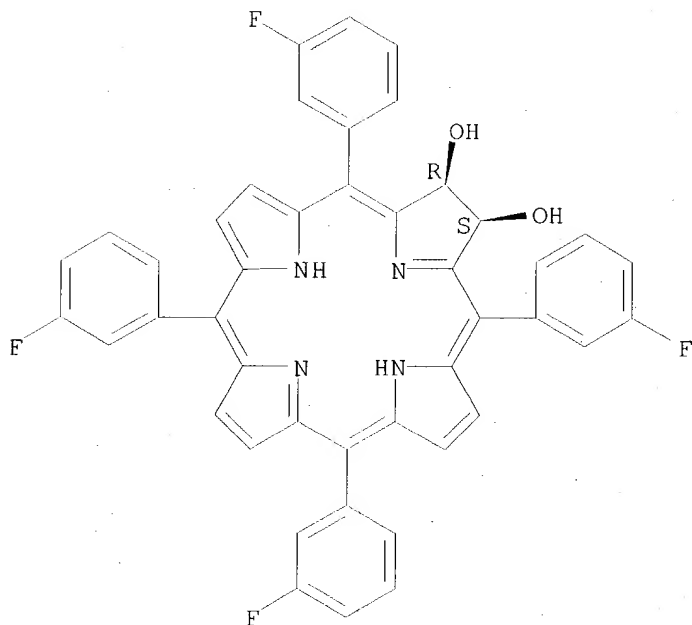


PAGE 2-A



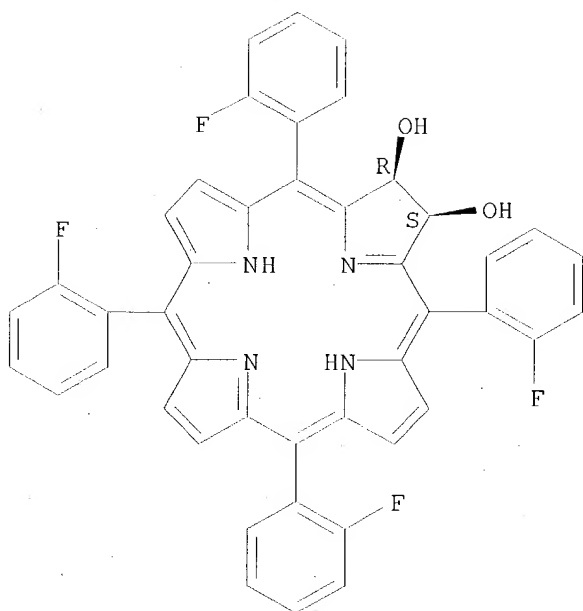
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, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 301336-70-9 USPATFULL
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(2-fluorophenyl)-7,8-dihydro-
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

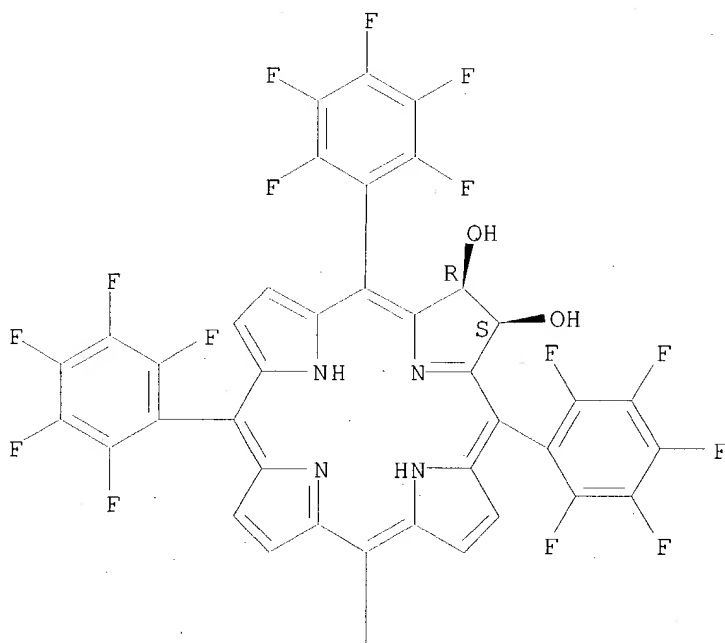
Relative stereochemistry.



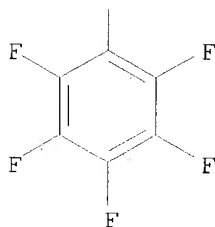
RN 301336-74-3 USPATFULL
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-
 tetrakis(pentafluorophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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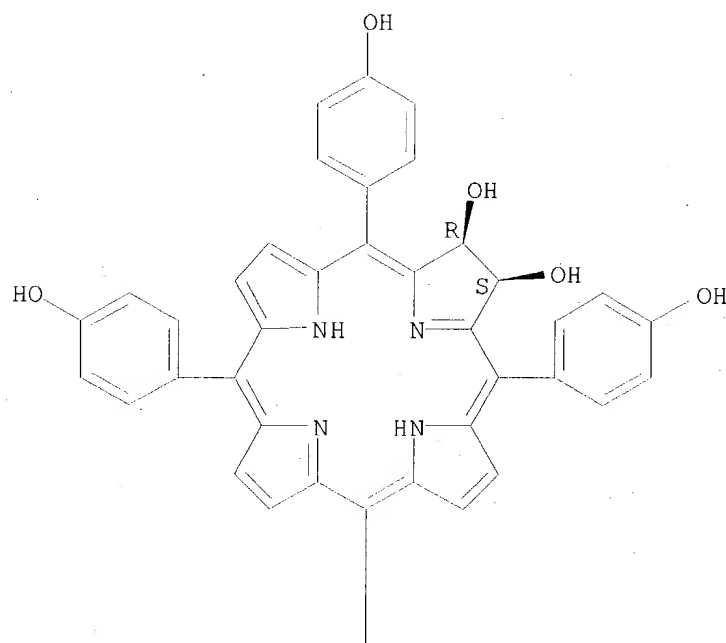
PAGE 2-A



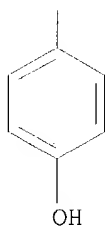
RN 301336-78-7 USPATFULL
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

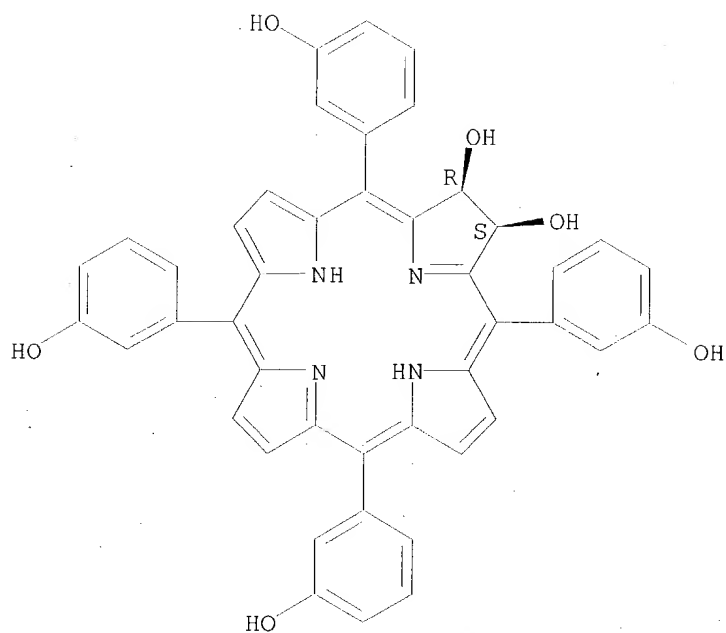


PAGE 2-A



RN 301336-82-3 USPATFULL
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-hydroxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

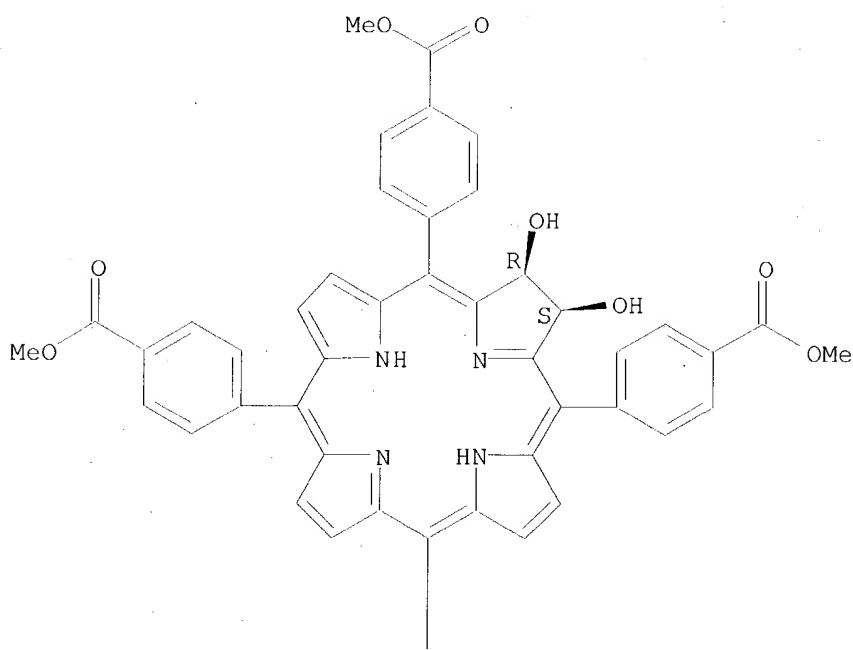
Relative stereochemistry.



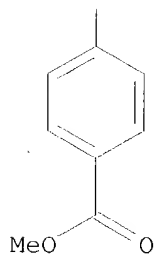
RN 301336-85-6 USPATFULL
 CN Benzoic acid, 4,4',4'',4'''-[(7R,8S)-7,8-dihydro-7,8-dihydroxy-21H,23H-porphine-5,10,15,20-tetrayl]tetrakis-, tetramethyl ester, rel- (9CI)
 (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



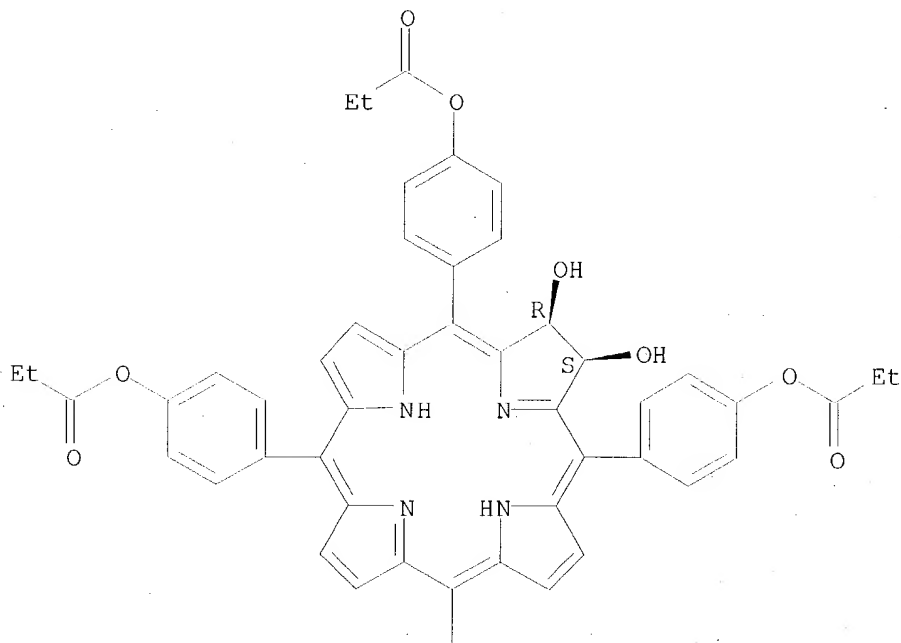
PAGE 2-A



RN 301336-88-9 USPATFULL
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis[4-(1-oxopropoxy)phenyl]-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

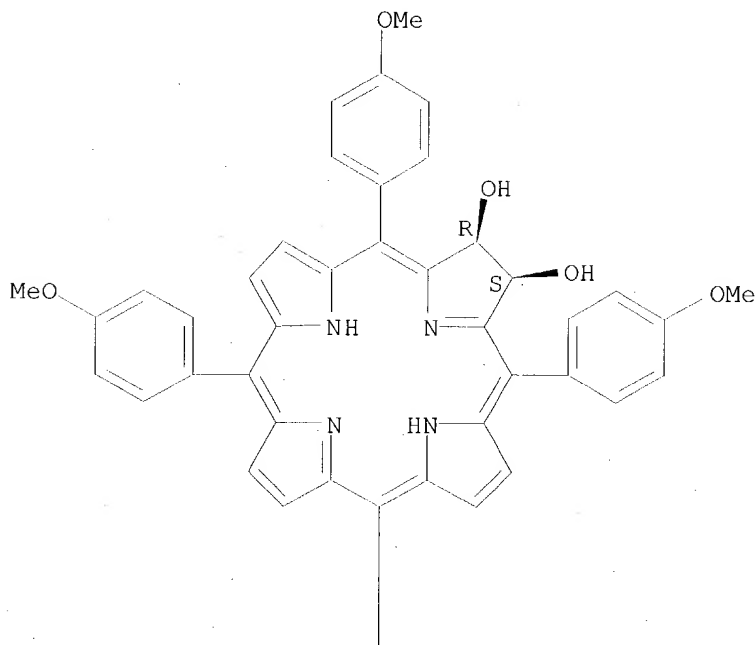
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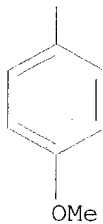
RN 301336-91-4 USPATFULL
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

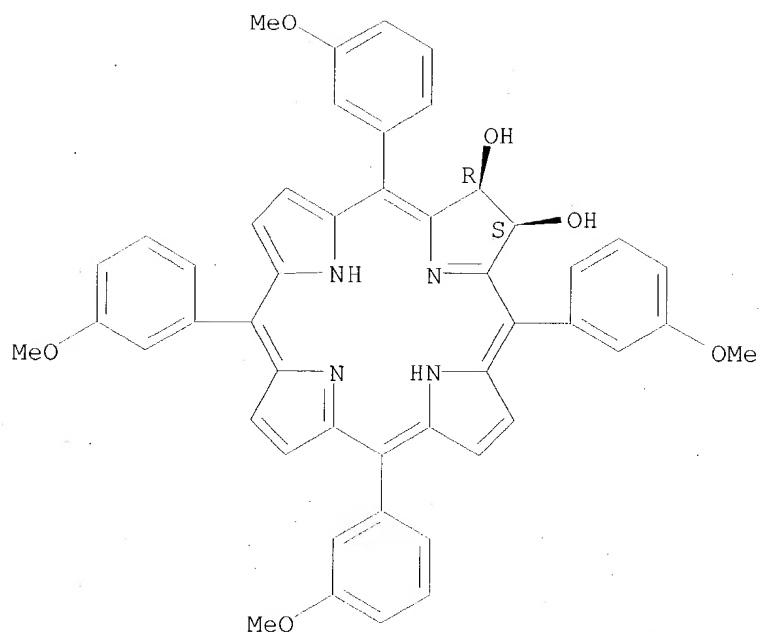


PAGE 2-A



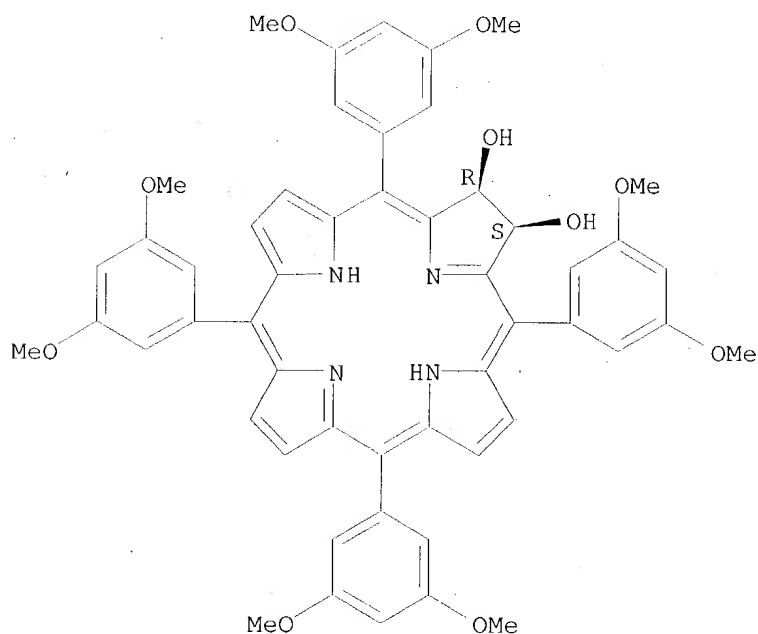
RN 301336-94-7 USPATFULL
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 301336-97-0 USPATFULL
 CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3,5-dimethoxyphenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

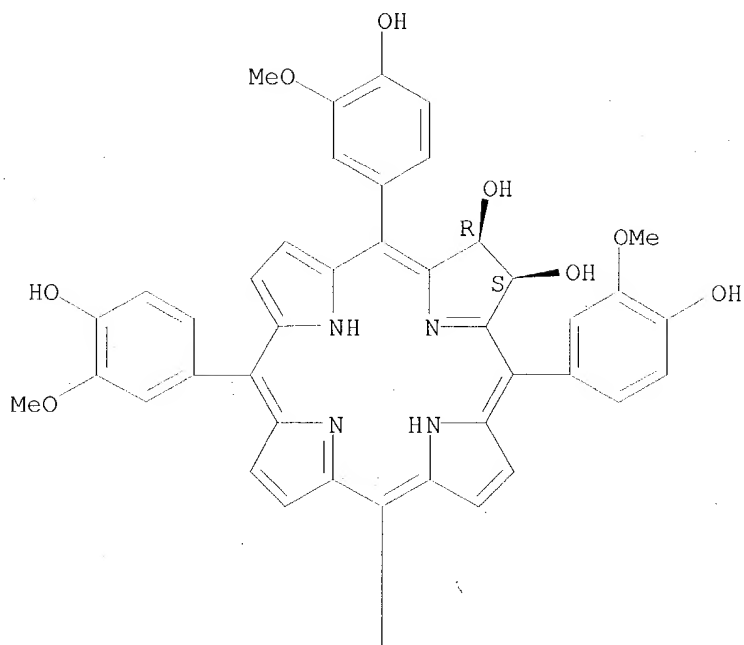
Relative stereochemistry.



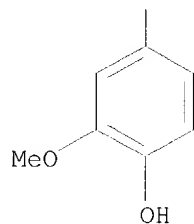
RN 301337-00-8 USPATFULL
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxy-3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



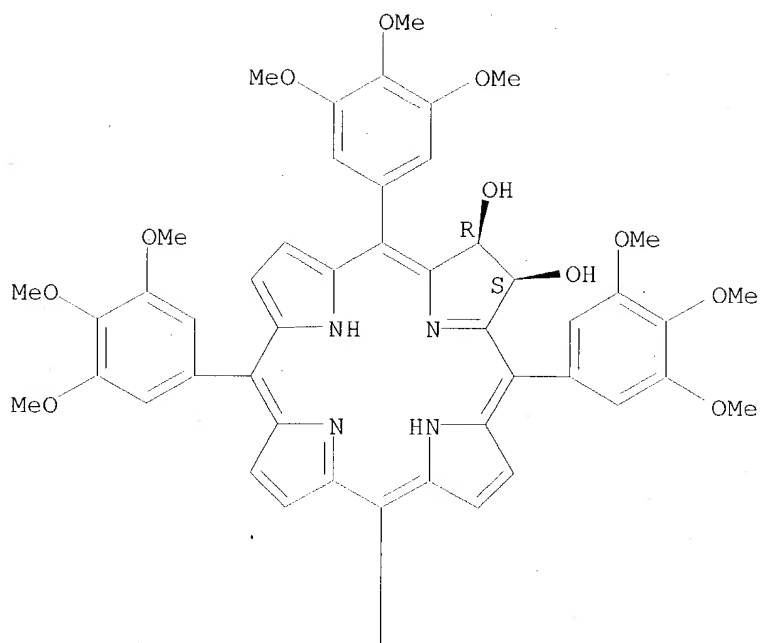
PAGE 2-A



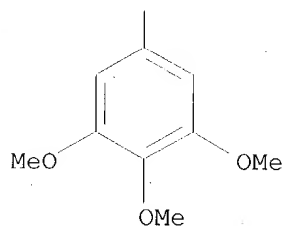
RN 301337-03-1 USPATFULL
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Relative stereochemistry.

PAGE 1-A

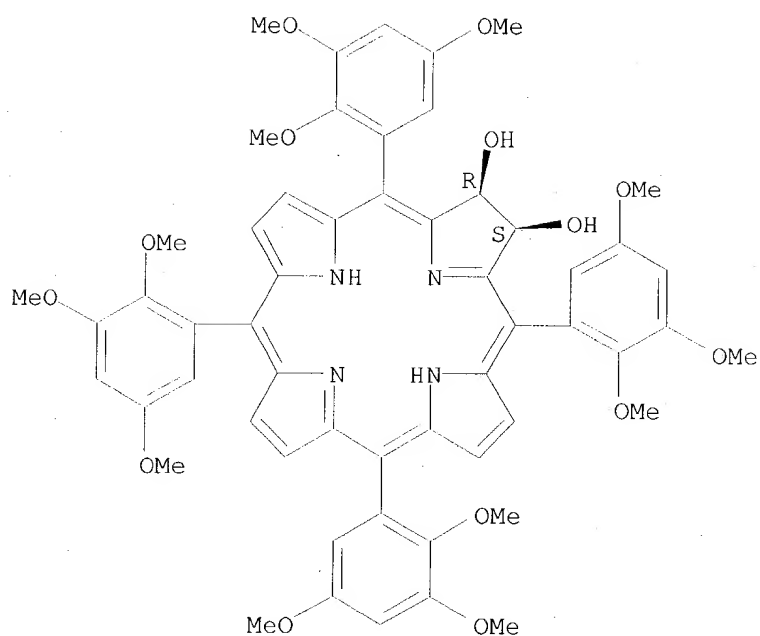


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RN 301337-05-3 USPATFULL
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Relative stereochemistry.

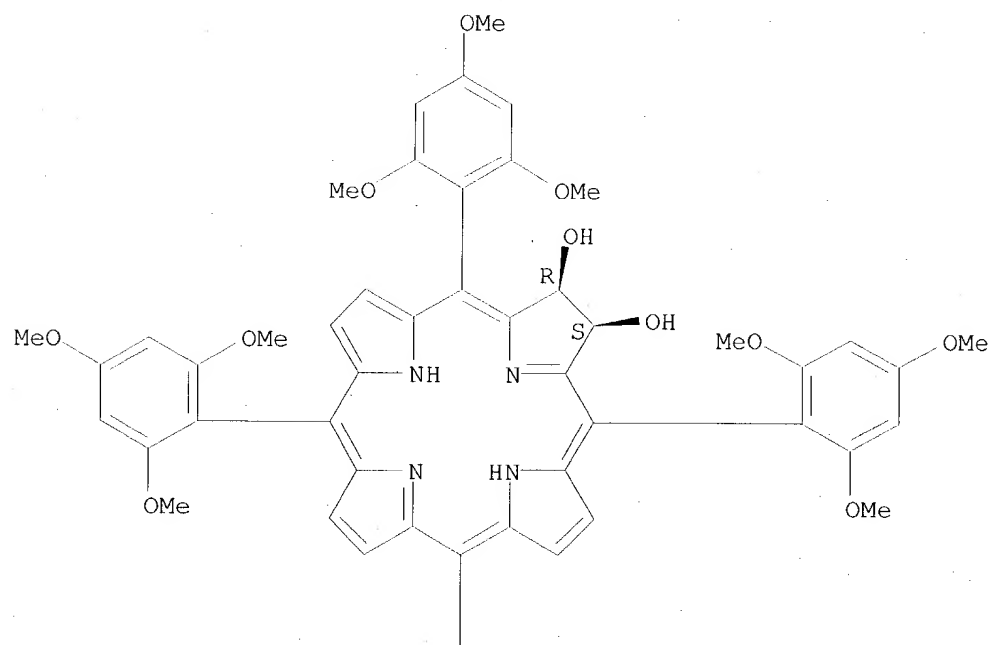


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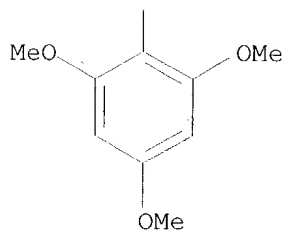
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,4,6-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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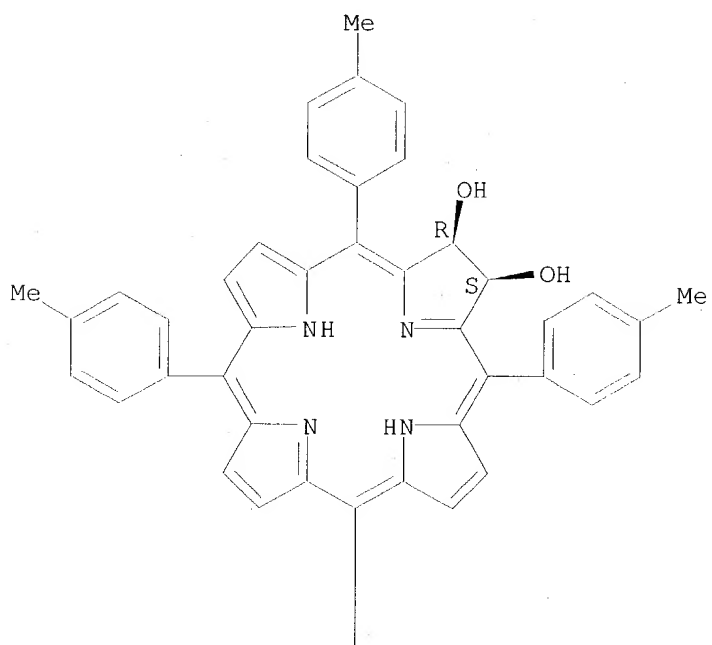
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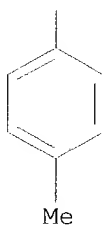
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Relative stereochemistry.

PAGE 1-A



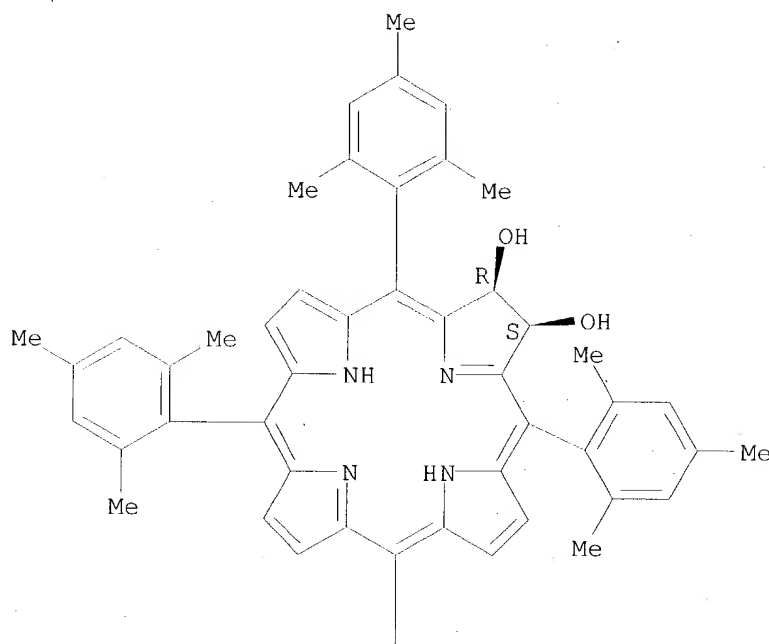
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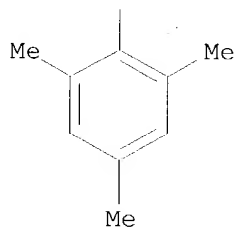
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Relative stereochemistry.

PAGE 1-A



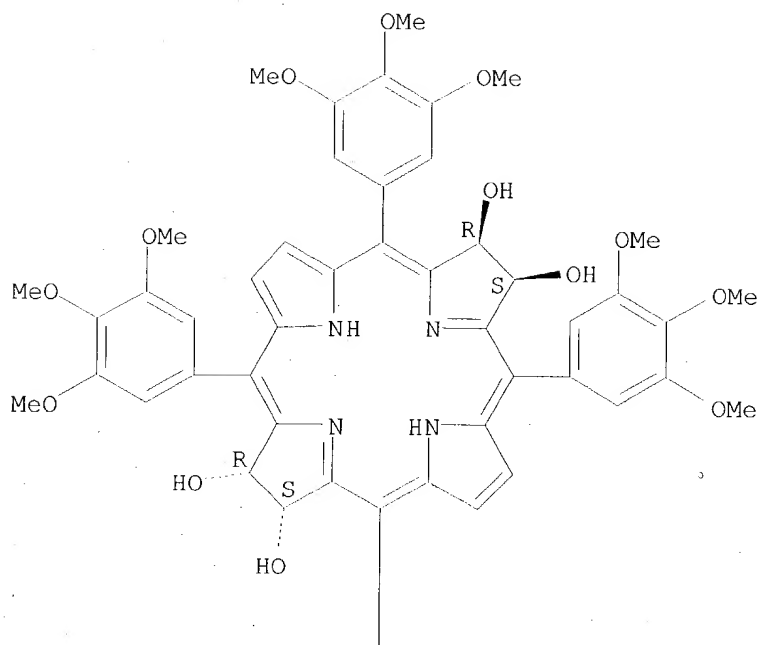
PAGE 2-A



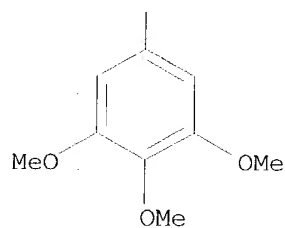
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Relative stereochemistry.

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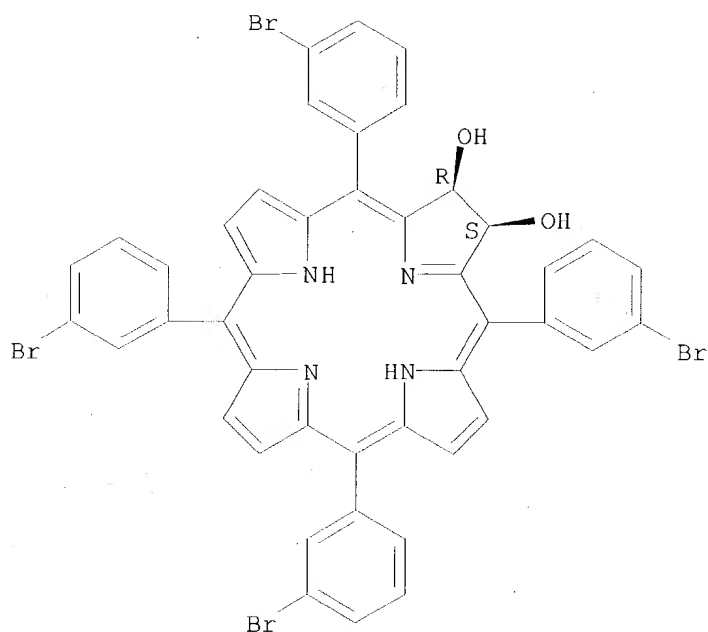


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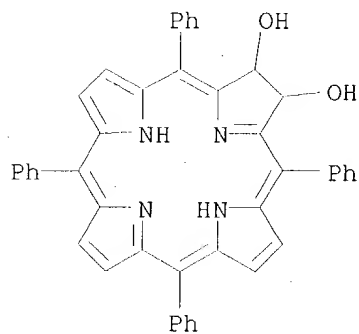


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Relative stereochemistry.

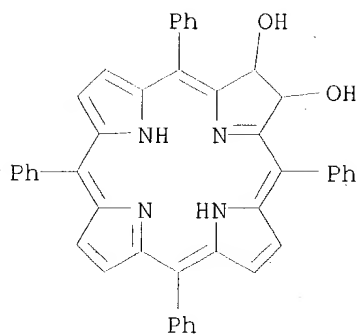


RN 301530-01-8 USPATFULL
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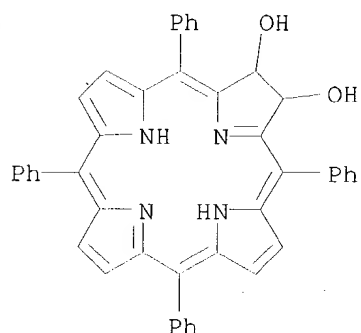
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RN 301530-02-9 USPATFULL
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D1-OH

RN 301530-03-0 USPATFULL
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5(or 15)-(4-nitrophenyl)-
 10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)



D1-NO2

L56 ANSWER 2 OF 3 USPATFULL on STN
 AN 1998:135229 USPATFULL
 TI Methods to prepare $\beta\beta'$ -dihydroxy meso-substituted chlorins,
 isobacteriochlorins and bacteriochlorins
 IN Dolphin, David, Vancouver, Canada
 Bruckner, Christian, Vancouver, Canada
 PA The University of British Columbia, Vancouver, Canada (non-U.S.
 corporation)
 PI US 5831088 19981103
 AI US 1997-853115 19970508 (8)
 RLI Division of Ser. No. US 1994-329577, filed on 26 Oct 1994, now patented,
 Pat. No. US 5648485
 DT Utility
 FS Granted
 EXNAM Primary Examiner: Shah, Mukund J.; Assistant Examiner: Sripada,
 Pavanaram K.
 LREP Murashige, Kate H.
 CLMN Number of Claims: 15
 ECL Exemplary Claim: 1
 DRWN 5 Drawing Figure(s); 5 Drawing Page(s)
 LN.CNT 1408

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A β,β' -dihydroxy meso-substituted chlorin, bacteriochlorin or isobacteriochlorin compound having the formula (I) or (II): ##STR1## wherein M is a metal. A novel method for synthesizing the compound of formula (I) or (II) comprises the steps of:

- osmylating a β,β' -unsubstituted, meso-substituted porphyrin to form an osmate ester at the β,β' -position, and
- reducing the osmate ester to form the corresponding β,β' -dihydroxy meso-substituted chlorin, bacteriochlorin or isobacteriochlorin of formula (I) or (II).

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

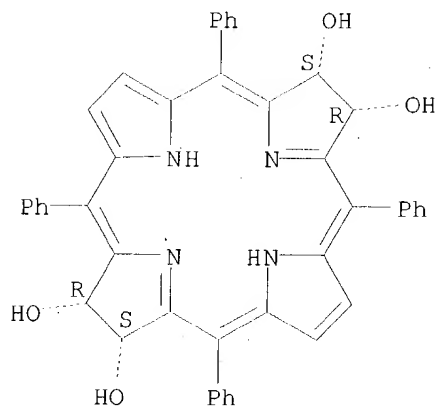
IT 172805-94-6P 172925-98-3P

(preparation of dihydroxychlorins for use in photodynamic therapy)

RN 172805-94-6 USPATFULL

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17R,18S)-rel- (9CI) (CA INDEX NAME)

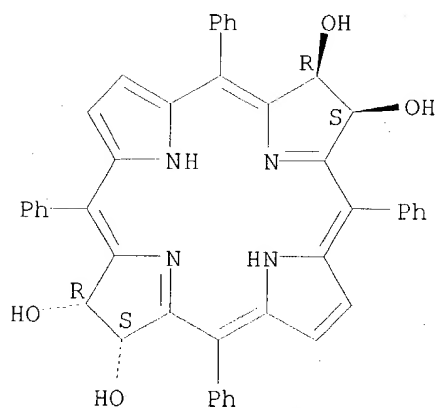
Relative stereochemistry.



RN 172925-98-3 USPATFULL

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L56 ANSWER 3 OF 3 USPATFULL on STN
 AN 97:61812 USPATFULL
 TI β , β -dihydroxy meso-substituted chlorins, isobacteriochlorins,
 and bacteriochlorins
 IN Dolphin, David, Vancouver, Canada
 Bruckner, Christian, Vancouver, Canada
 PA University of British Columbia, Vancouver, Canada (non-U.S. corporation)
 PI US 5648485 19970715
 AI US 1994-329577 19941026 (8)
 DT Utility
 FS Granted
 EXNAM Primary Examiner: Shah, Mukund J.; Assistant Examiner: Sripada,
 Pavanaram K.
 LREP Morrison & Foerster LLP
 CLMN Number of Claims: 12
 ECL Exemplary Claim: 1
 DRWN 5 Drawing Figure(s); 5 Drawing Page(s)
 LN.CNT 1393

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A β , β' -dihydroxy meso-substituted chlorin, bacteriochlorin or
 isobacteriochlorin compound having the formula (I) or (II): ##STR1##
 wherein M is a metal. A novel method for synthesizing the compound of
 formula (I) or (II) comprises the steps of:

a. osmylating a β , β' -unsubstituted, meso-substituted porphyrin
 to form an osmate ester at the β , β' -position, and

b. reducing the osmate ester to form the corresponding
 β , β' -dihydroxy meso-substituted chlorin, bacteriochlorin or
 isobacteriochlorin of formula (I) or (II).

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

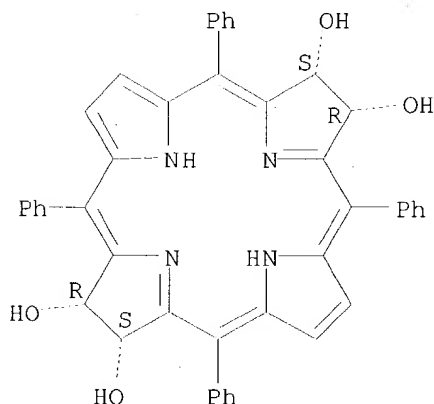
IT 172805-94-6P 172925-98-3P

(preparation of dihydroxychlorins for use in photodynamic therapy)

RN 172805-94-6 USPATFULL

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-
 tetraphenyl-, (7R,8S,17R,18S)-rel- (9CI) (CA INDEX NAME)

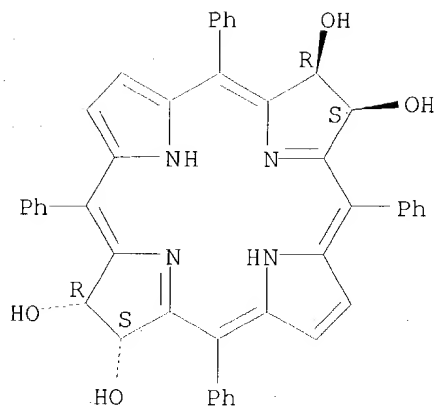
Relative stereochemistry.



RN 172925-98-3 USPATFULL

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-
 tetraphenyl-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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L55 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:943390 HCAPLUS

DN 138:137068

ED Entered STN: 13 Dec 2002

TI Free Base meso-Tetraaryl-morpholinochlorins and Porpholactone from meso-Tetraaryl-2,3-dihydroxy-chlorin

AU McCarthy, Jason R.; Jenkins, Hilary A.; Brueckner, Christian

CS Department of Chemistry, University of Connecticut, Storrs, CT, 06269-3060, USA

SO Organic Letters (2003), 5(1), 19-22

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

CC 26-7 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 28, 75

OS CASREACT 138:137068

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB Meso-Tetraaryl-2,3-dihydroxychlorins, e.g. I, were converted in one step to novel free base macrocyclic meso-tetraaryl-2,3-dialkoxy-2a-oxa-2a-homoporphyrins, e.g. II. Their bathochromically shifted chlorin-type UV-vis spectra indicate the presence of a nonplanar chromophore. The structure of meso-tetratolyldiethoxymorpholinochlorin III (R = p-tolyl), as determined by X-ray crystallog., was found to be largely planar, suggesting significant conformational flexibility of these macrocycles. Oxidation of diol I with MnO₄ generates known porpholactone IV in high yields.
- ST meso tetraarylmorpholinochlorin stereoselective synthesis tetraaryldihydroxychlorin dihydroxylation oxidative diol cleavage; ring closure heterocyclization meso tetraarylmorpholinochlorin stereoselective synthesis; porpholactone prepn oxidn meso tetraaryldihydroxychlorin; crystal structure free base meso tetraarylmorpholinochlorin; UV VIS spectra free base meso tetraarylmorpholinochlorin; chlorin tetraarylmorpholino stereoselective synthesis tetraaryldihydroxychlorin
- IT Porphyrins
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(chlorins; free-base meso-tetraarylmorpholinochlorins and porpholactone from meso-tetraaryl-2,3-dihydroxy-chlorin)
- IT Heterocyclization
Hydroxylation
(free-base meso-tetraarylmorpholinochlorins from meso-tetraaryl-2,3-dihydroxy-chlorins via)
- IT Crystal structure
(of a free-base meso-tetraarylmorpholinochlorin)
- IT UV and visible spectra
(of free-base meso-tetraarylmorpholinochlorins)
- IT Stereoselective synthesis
(of free-base meso-tetraarylmorpholinochlorins from meso-tetraaryl-2,3-dihydroxy-chlorins)
- IT Bond cleavage
(oxidative; free-base meso-tetraarylmorpholinochlorins from meso-tetraaryl-2,3-dihydroxy-chlorins via)
- IT Oxidation
(porpholactone from meso-tetraaryl-2,3-dihydroxychlorin via)
- IT 493038-30-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; free-base meso-tetraarylmorpholinochlorins and porpholactone from meso-tetraaryl-2,3-dihydroxy-chlorin)
- IT 64-17-5, Ethanol, reactions 67-63-0, Isopropanol, reactions 165336-18-5 **301337-10-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(free-base meso-tetraarylmorpholinochlorins and porpholactone from meso-tetraaryl-2,3-dihydroxy-chlorin)
- IT 493038-27-0P 493038-28-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(free-base meso-tetraarylmorpholinochlorins and porpholactone from meso-tetraaryl-2,3-dihydroxy-chlorin)
- IT 493038-29-2P 493038-31-6P 493038-32-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(free-base meso-tetraarylmorpholinochlorins and porpholactone from meso-tetraaryl-2,3-dihydroxy-chlorin)
- RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
- RE
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IT 301337-10-0

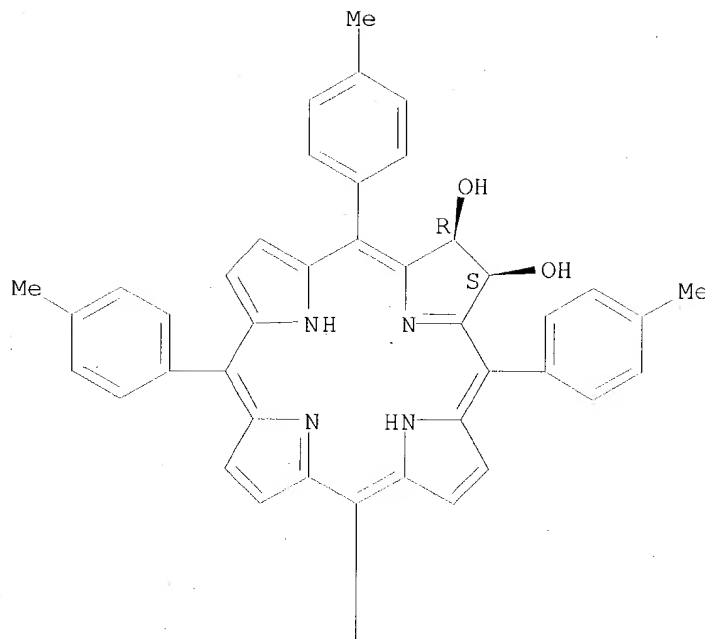
RL: RCT (Reactant); RACT (Reactant or reagent)
(free-base meso-tetraarylmorpholinochlorins and porpholactone from
meso-tetraaryl-2,3-dihydroxy-chlorin)

RN 301337-10-0 HCAPLUS

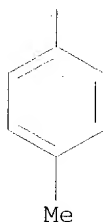
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methylphenyl)-
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



L55 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:749172 HCAPLUS
DN 138:39122
ED Entered STN: 03 Oct 2002
TI Evaluation of tetraphenyl-2,3-dihydroxychlorins as potential
photosensitizers
AU **MacAlpine, Jill K.**; Boch, Ron; **Dolphin, David**
CS Department of Chemistry, University of British Columbia, Vancouver, BC,
V6T 1Z1, Can.
SO Journal of Porphyrins and Phthalocyanines (2002), 6(2), 146-155
CODEN: JPPHFZ; ISSN: 1088-4246
PB Society of Porphyrins & Phthalocyanines
DT Journal
LA English
CC 26-7 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1
OS CASREACT 138:39122
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB A series of β,β -dihydroxychlorins, e.g. I, derived from meso-tetraphenylporphyrins (TPPs) have been synthesized. Their in vitro cytotoxicity has been measured and compared to BPDMA (verteporfin, II). Under the assay conditions BPDMA had an LD50 (LD to kill 50% of cells) value of 0.007 μM (5 ng/mL). The LD50 values for the TPP derivs. varied from 1.7×10^{-2} to 9.9 μM depending upon the substituents and their position on the Ph groups. One example of the dihydroxychlorin prepared from unsubstituted 5,15-diphenylporphyrin was examined and this exhibited an LD50 of 2.4×10^{-3} μM !
- ST tetraphenyldihydroxychlorin prepn dihydroxylation tetraphenylporphyrin photosensitizer photodynamic therapy tetraphenyldihydroxy chlorin; antitumor agent cancer dark toxicity phototoxicity tetraphenyldihydroxychlorin tetraphenyldihydroxy chlorin
- IT Porphyrins
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(chlorins; evaluation of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)
- IT Toxicity
(dark; of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)
- IT Antitumor agents
Human
Neoplasm
Photodynamic therapy
Photosensitizers (pharmaceutical)
(evaluation of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)
- IT Phototoxicity
(of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)
- IT Porphyrins
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tetraphenyl-2,3-dihydroxychlorins from)
- IT 129497-78-5, Verteporfin
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(evaluation of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)
- IT 165336-18-5P 165336-21-0P 301336-58-3P
301336-61-8P 301336-66-3P 301336-70-9P
301336-74-3P 301336-78-7P 301336-82-3P
301336-85-6P 301336-91-4P 301336-94-7P
301336-97-0P 301337-00-8P 301337-03-1P
301337-10-0P 301337-13-3P 301337-16-6P 301337-19-9P
301338-12-5P 478415-82-6P 478415-83-7P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(evaluation of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)
- IT 917-23-7 14527-51-6 22112-78-3 22112-79-4 22112-80-7 22112-83-0
22112-89-6 25440-14-6 27185-62-2 29114-93-0 29162-73-0
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68772-71-4 74684-34-7 74684-35-8 87345-22-0 94317-94-9
110452-48-7 185143-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(evaluation of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)
- IT 301336-88-9P
RL: SPN (Synthetic preparation); PREP (Preparation)

(evaluation of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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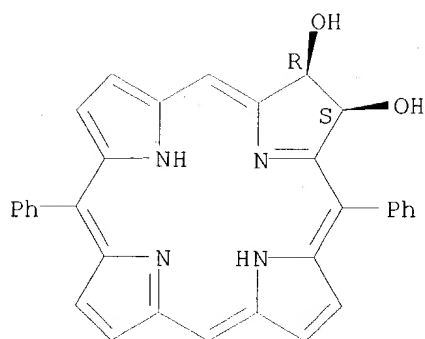
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301337-00-8P 301337-03-1P 301337-10-0P
301337-13-3P 301338-12-5P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(evaluation of tetraphenyl-2,3-dihydroxychlorins as potential photosensitizers)

RN 165336-21-0 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-diphenyl-, (7R,8S)-rel- (9CI)
(CA INDEX NAME)

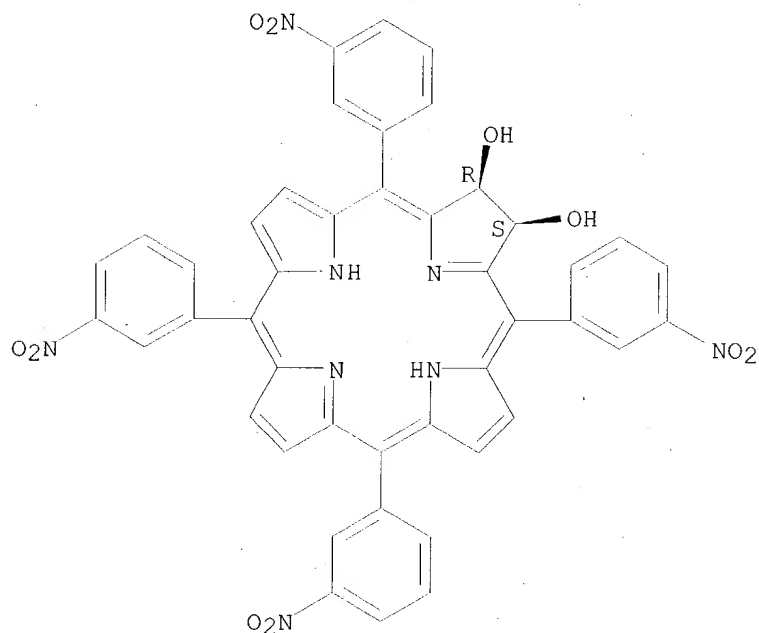
Relative stereochemistry.



RN 301336-58-3 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-nitrophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

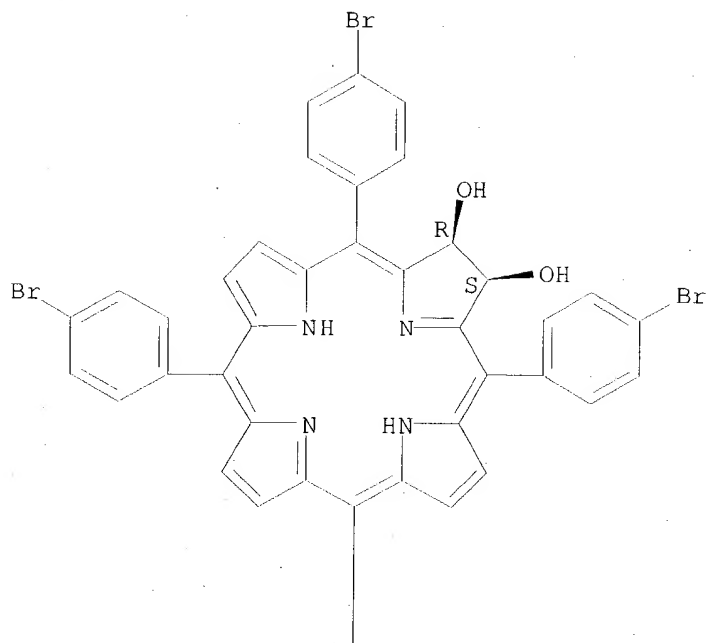


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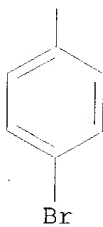
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(4-bromophenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



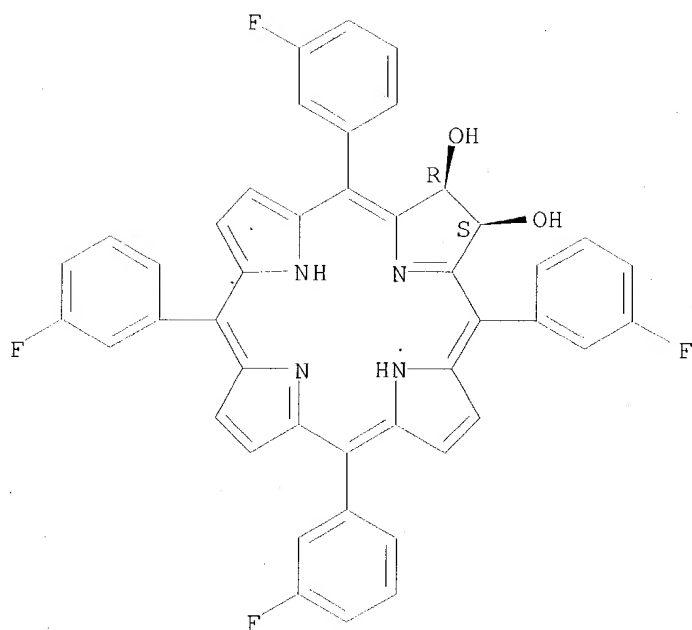
PAGE 2-A



RN 301336-66-3 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3-fluorophenyl)-7,8-dihydro-
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

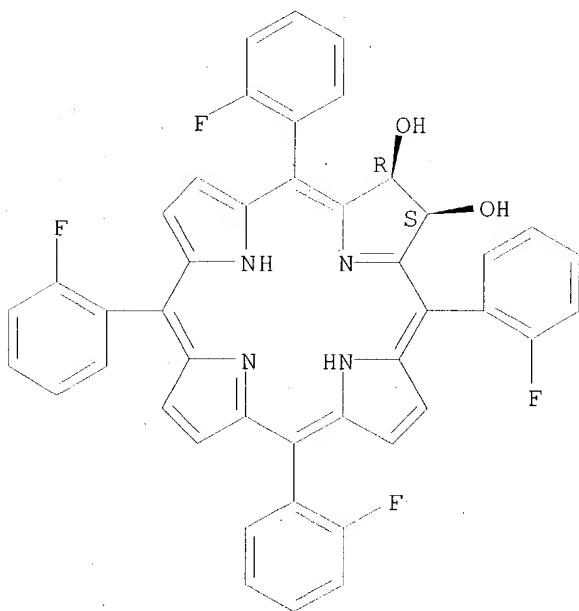
Relative stereochemistry.



RN 301336-70-9 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(2-fluorophenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

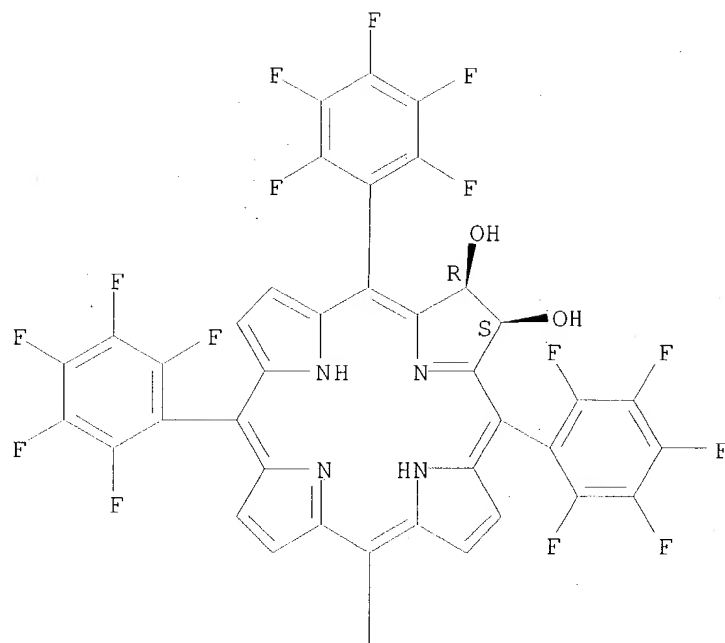


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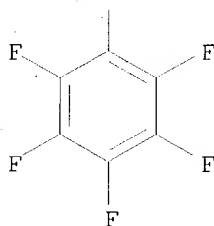
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(pentafluorophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

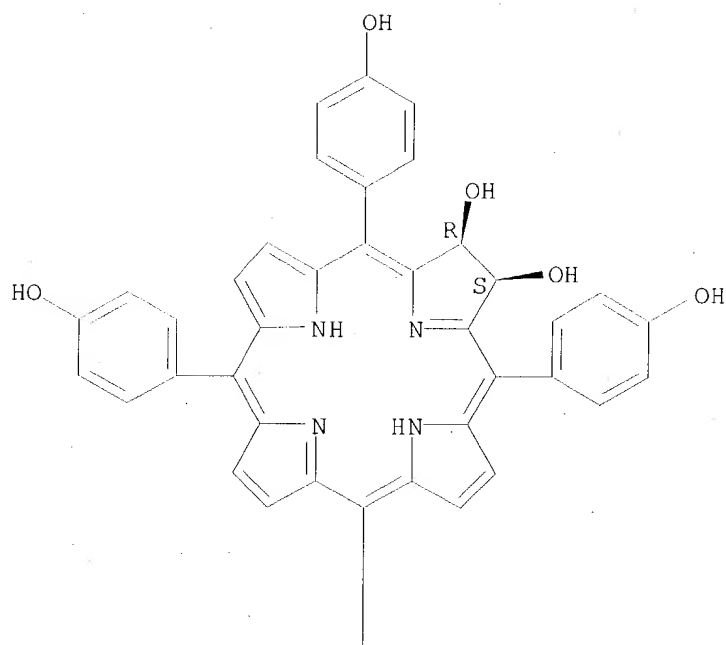


RN 301336-78-7 HCAPLUS

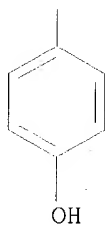
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

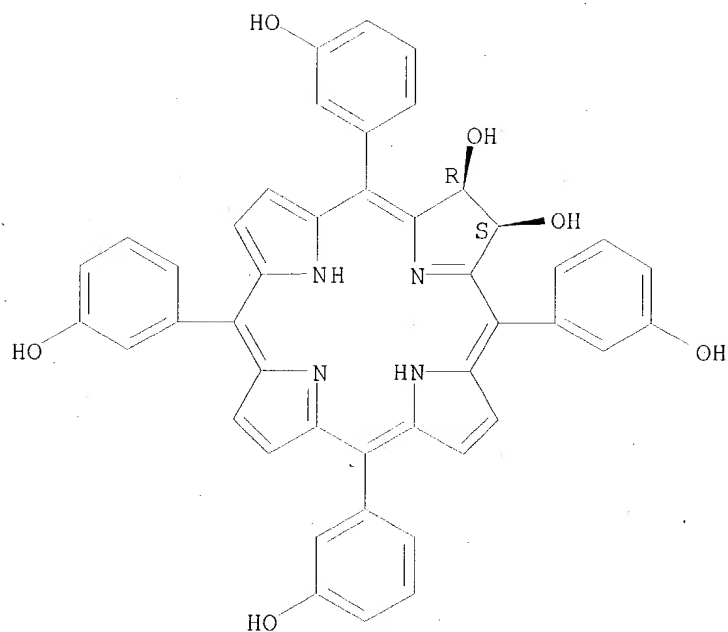


PAGE 2-A



RN 301336-82-3 HCAPLUS
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-hydroxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

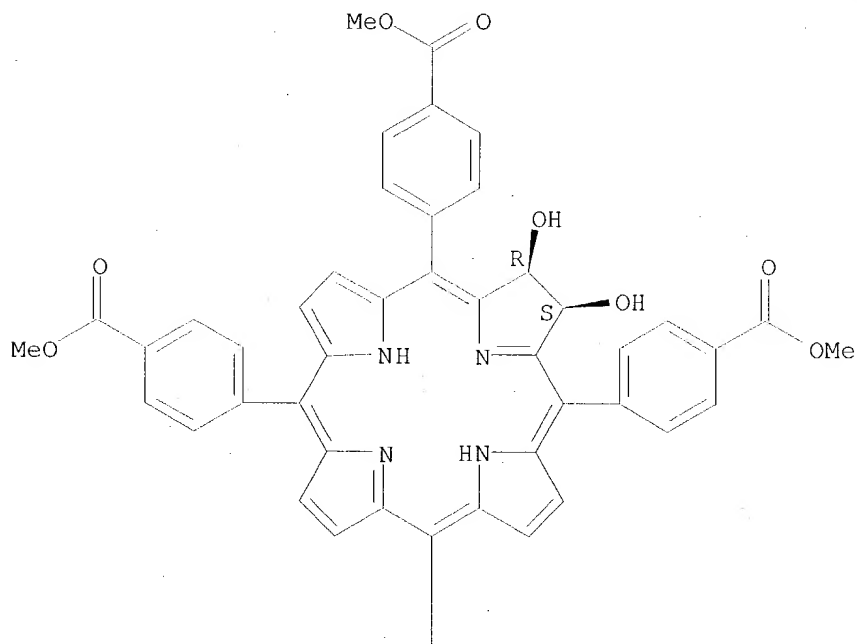


RN 301336-85-6 HCAPLUS

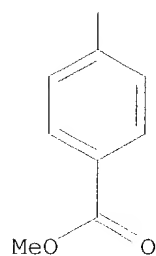
CN Benzoic acid, 4,4',4'',4'''-[(7R,8S)-7,8-dihydro-7,8-dihydroxy-21H,23H-porphine-5,10,15,20-tetrayl]tetrakis-, tetramethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



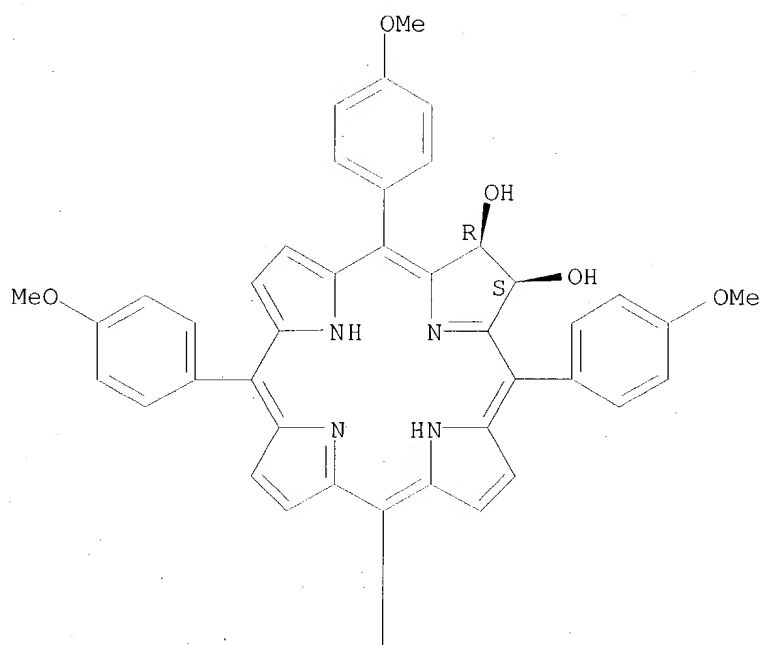
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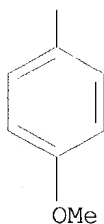
RN 301336-91-4 HCAPLUS
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

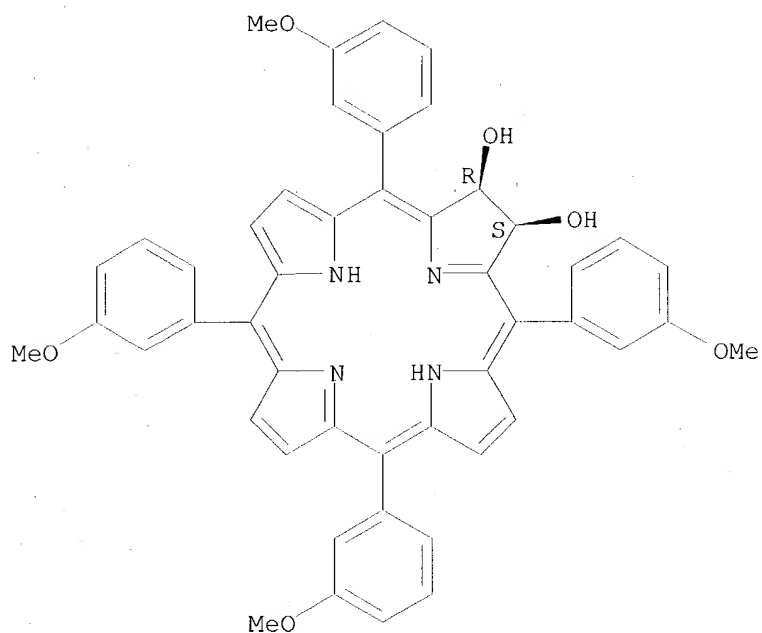


PAGE 2-A



RN 301336-94-7 HCAPLUS
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

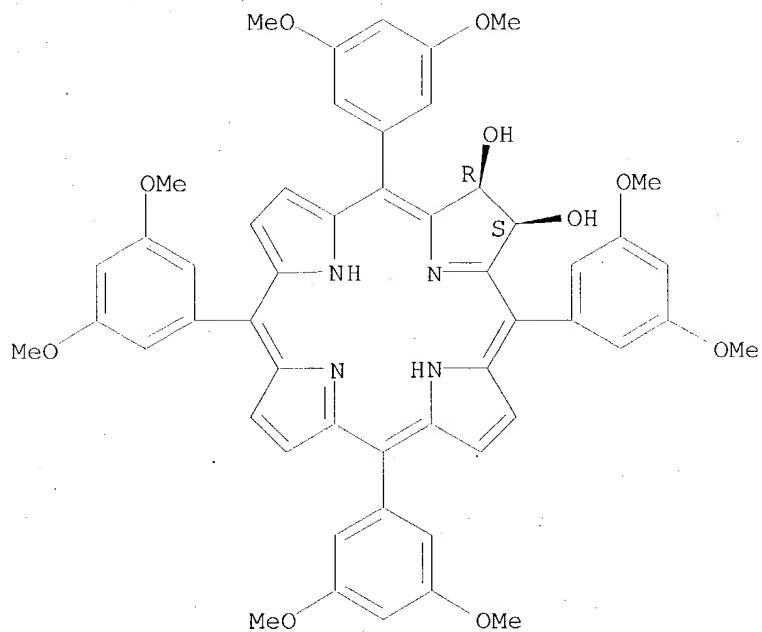
Relative stereochemistry.



RN 301336-97-0 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3,5-dimethoxyphenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

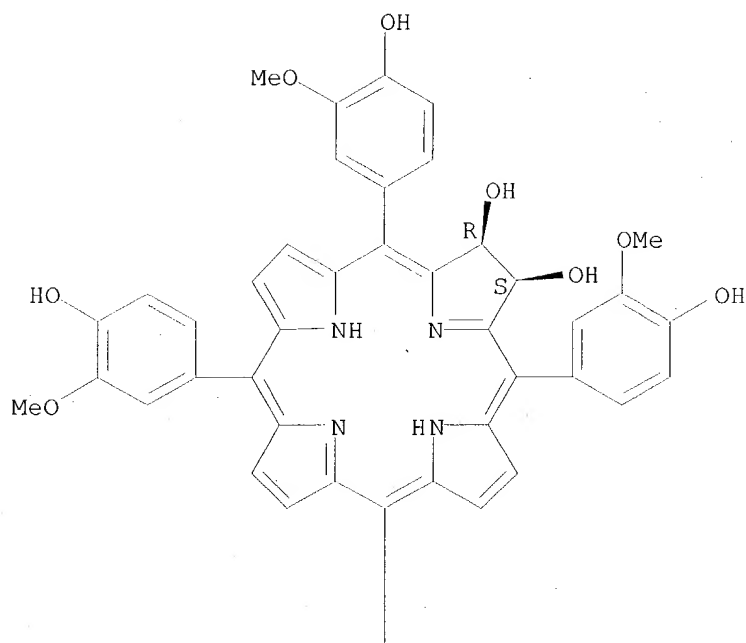


RN 301337-00-8 HCAPLUS

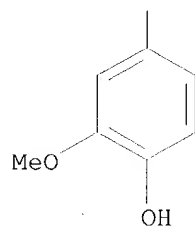
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxy-3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



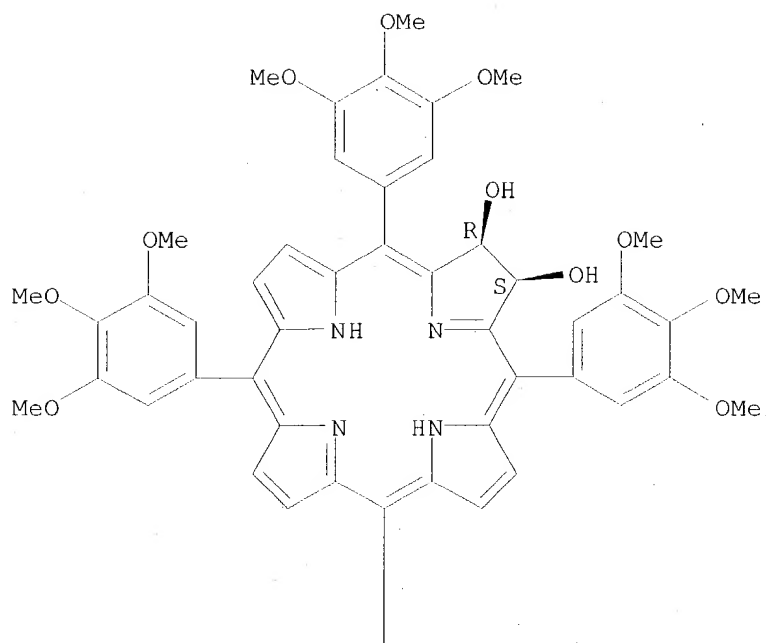
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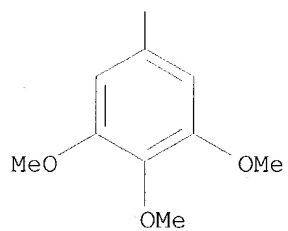
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CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3,4,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



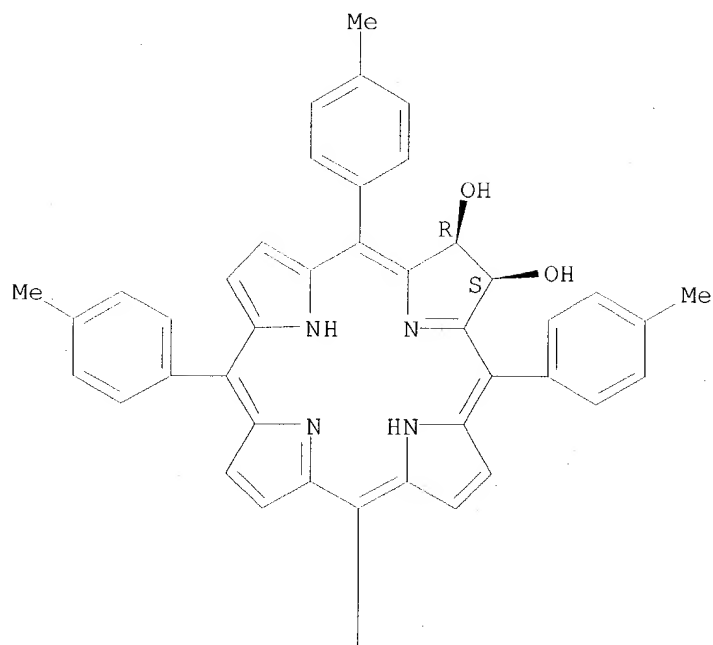
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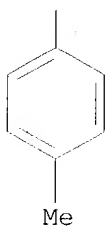
RN 301337-10-0 HCAPLUS
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methylphenyl)-
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



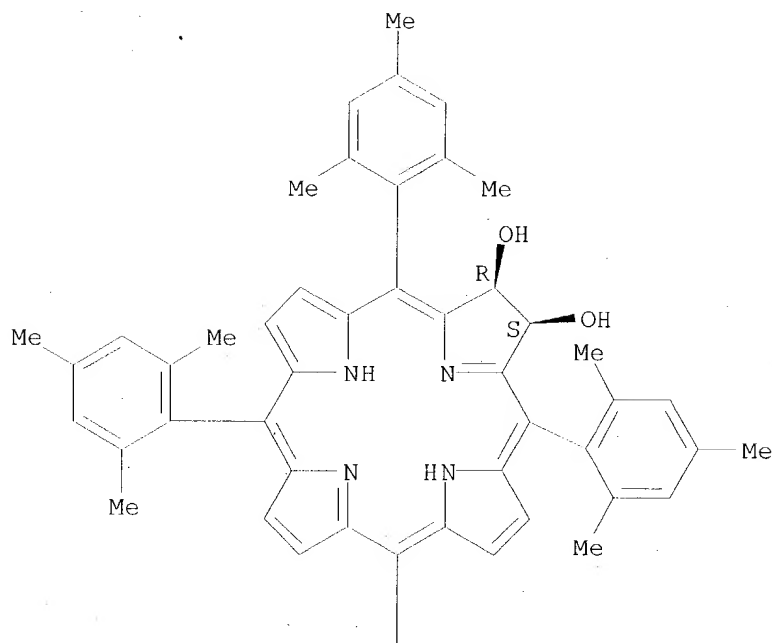
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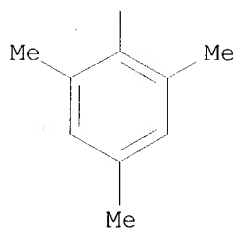
RN 301337-13-3 HCAPLUS
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



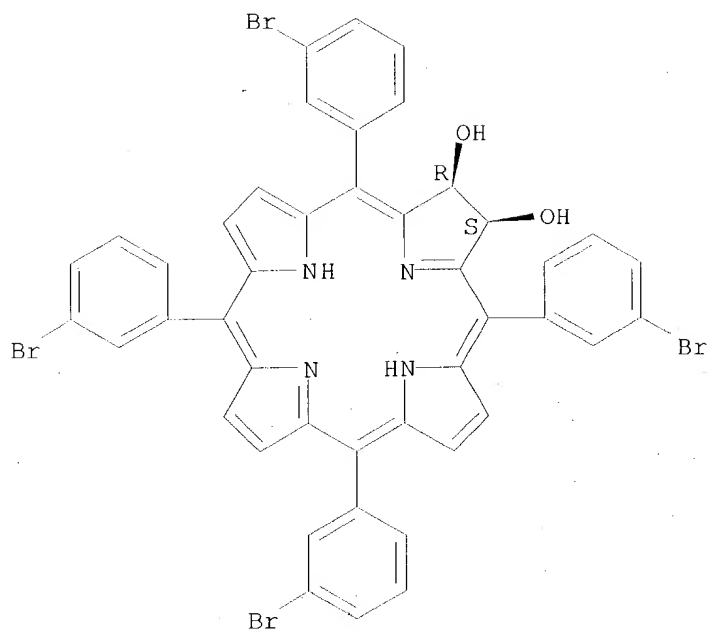
PAGE 2-A



RN 301338-12-5 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3-bromophenyl)-7,8-dihydro-
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

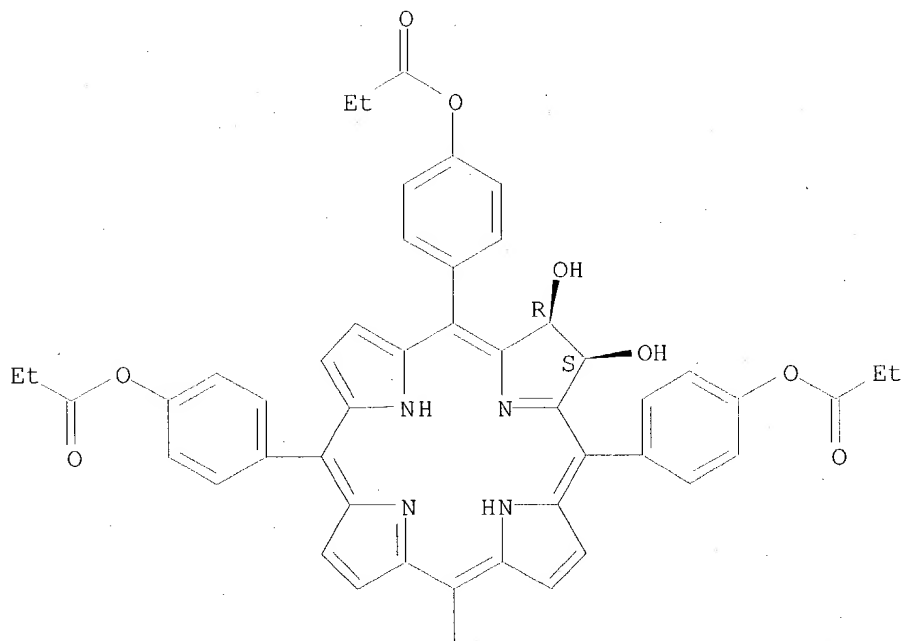


RL: SPN (Synthetic preparation); PREP (Preparation)
(evaluation of tetraphenyl-2,3-dihydroxychlorins as potential
photosensitizers)

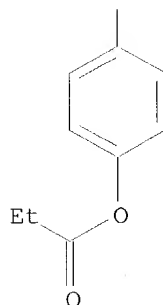
21H, 23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis[4-(1-oxopropoxy)phenyl]-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



L55 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 2001:501958 HCAPLUS
 DN 135:288614
 ED Entered STN: 12 Jul 2001
 TI Synthesis and Photodynamic Action of Diphenyl-2,3-dihydroxychlorin: a
 Potential Tumor Photosensitizer
 AU Wang, T. Y.; Liu, H. L.; Chen, J. R.; Liu, F. G.; Gu, Y.; Ma, J. S.
 CS Institute of Chemistry, Center for Molecular Science, Chinese Academy of
 Sciences, Beijing, 100080, Peop. Rep. China
 SO Bioorganic & Medicinal Chemistry Letters (2001), 11(15), 2049-2052
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 CC 26-7 (Biomolecules and Their Synthetic Analogs)
 Section cross-reference(s): 1
 OS CASREACT 135:288614
 AB The synthesis, photophys. properties of diphenyl-2,3-dihydroxychlorin
 (DPCOH) and its photocytotoxicity to tumor cells are described. DPCOH
 exhibits photodynamic activity in terms of type I and type II mechanisms
 under irradiation. The quantum yield of 102 in CHCl₃ is 0.7. For the
 photocytotoxicity to tumor cells, DPCOH proved to be 200 times more potent
 than HPD, and the dark toxicity is low (dark IC₉₀>32 µg/mL).
 ST chlorin diphenyldihydroxy prepn photodynamic action; photocytotoxicity
 chlorin diphenyldihydroxy prepn
 IT Phototoxicity
 (photocytotoxicity; synthesis and photodynamic action of
 di-phenyl-2,3-dihydroxychlorin)
 IT Photodynamic action
 (synthesis and photodynamic action of di-phenyl-2,3-dihydroxychlorin)
 IT Photosensitizers (pharmaceutical)
 (synthesis of di-phenyl-2,3-dihydroxychlorin as a potential tumor
 photosensitizer)
 IT **165336-21-0P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological
 study); PREP (Preparation)
 (synthesis and photodynamic action of di-phenyl-2,3-dihydroxychlorin)
 IT 100-52-7, Benzaldehyde, reactions 109-97-7, Pyrrole
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis and photodynamic action of di-phenyl-2,3-dihydroxychlorin)
 IT 22112-89-6P 107798-98-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (synthesis and photodynamic action of di-phenyl-2,3-dihydroxychlorin)

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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IT 165336-21-0P

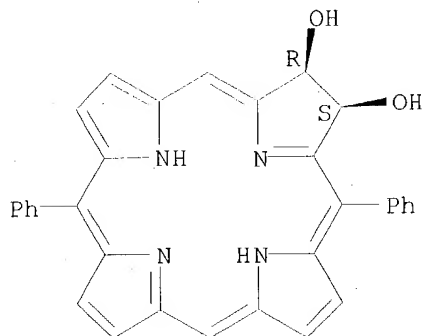
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and photodynamic action of di-phenyl-2,3-dihydroxychlorin)

RN 165336-21-0 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-diphenyl-, (7R,8S)-rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



L55 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:298484 HCAPLUS

DN 135:86084

ED Entered STN: 27 Apr 2001

TI Cavitand-Porphyrins

AU Starnes, Stephen D.; Rudkevich, Dmitry M.; Rebek, Julius, Jr.

CS The Skaggs Institute for Chemical Biology and The Department of Chemistry,
The Scripps Research Institute, La Jolla, CA, 92037, USA

SO Journal of the American Chemical Society (2001), 123(20), 4659-4669
CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 26

OS CASREACT 135:86084

AB The synthesis and characterization of new nanoscale container mols. 7 and 8 are described. They are covalent hybrids of deepened, self-folding cavitands and metalloporphyrins. In receptor 7, the Zn-porphyrin wall is directly built onto the cavitand skeleton. Host 8 features a large unimol. cavity containing two cavitands attached with the Zn-porphyrin wall. Its dimensions, .apprx.10 + 25 Å, place it among the largest synthetic hosts prepared to date. Adamantyl- and pyridyl-containing guests 14-20 of various lengths were prepared and used to determine the hosts' binding abilities in solution using UV/visible and 1H NMR spectroscopy. Intramol. hydrogen bonds at the upper rims of the cavitands resist the unfolding of the inner cavities and thereby increase the energetic barrier to guest exchange. The exchange is slow on the NMR time scale (at ≤300 K), and kinetically stable complexes result. When the cavities and metalloporphyrins participate simultaneously in the binding event, very high affinities for guests are found (-ΔG295 up to 10 kcal mol⁻¹ in toluene), to which the porphyrin fragments contribute significantly (-ΔG295 up to 6 kcal mol⁻¹). The pairwise selection of two different guests by mol. container 8 is reported, and the termol. complex formed raises the possibility of metal-catalyzed bimol. reactions in these containers.

ST zinc porphyrin cavitand prepn inclusion

IT Formation constant

(association constant; preparation and host-guest binding study of zinc cavitand-porphyrin complexes)

IT Free energy of binding

Inclusion reaction

(preparation and host-guest binding study of zinc cavitand-porphyrin complexes)

IT Inclusion compounds

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and host-guest binding study of zinc cavitand-porphyrin complexes)

IT 880-52-4

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)

(host-guest binding with zinc cavitand-porphyrin host)

IT 286386-32-1P 347389-80-4P 347389-81-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and complexation with zinc)

IT 603112-32-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and host-guest binding study of zinc cavitand-porphyrin complexes)

IT 286386-28-5P 347388-87-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and host-guest binding study of zinc cavitand-porphyrin complexes with adamantyl- and pyridyl-containing guests)

IT 286386-50-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and host-guest binding with adamantyl- and pyridyl-containing guests)

IT 24813-21-6P 145958-66-3P 153872-62-9P 286386-40-1P 286386-42-3P

286386-44-5P 286386-46-7P 286386-48-9P 286386-49-0P 347143-86-6P

347143-87-7P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and host-guest binding with zinc cavitand-porphyrin host)

IT 347391-20-2P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)
 (preparation and toluene guest replacement with adamantyl- and
 pyridyl-containing guest)

IT 286386-51-4P 286386-53-6P 286386-55-8P 286386-57-0P 286386-59-2P
 286386-61-6P 286386-62-7P 286386-63-8P 286386-64-9P 347143-88-8P
 347391-60-0P 347391-89-3P 347391-95-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation in host-guest binding study of zinc cavitand-porphyrin
 complexes with adamantyl- and pyridyl-containing guests)

IT 347389-59-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 172805-94-6P 172925-98-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation, oxidation to porphyrintetrone and subsequent reaction to give
 zinc cavitand-porphyrin complex)

IT 100-46-9, Benzylamine, reactions 142-61-0, Hexanoyl chloride 768-94-5,
 1-Aminoadamantane 2094-72-6 3731-52-0, 3-(Aminomethyl)pyridine
 10400-19-8, 3-Pyridinecarbonyl chloride 17768-41-1, 1-
 (Aminomethyl)adamantane 19835-38-2 94413-66-8, 3,5-
 Bis(aminomethyl)pyridine 120067-55-2, 3-Pyridineacetyl chloride
 152656-95-6, 3-Pyridinepropanoyl chloride

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of adamantyl- and pyridyl-containing compds. for
 host-guest binding with zinc cavitand-porphyrin complex)

IT 27841-33-4, 1,2-Diamino-4,5-dimethoxybenzene

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of zinc benzopyrazinoporphyrin)

IT 917-23-7, meso-Tetraphenylporphyrin 94526-72-4 129515-14-6
 271790-46-6 286839-82-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of zinc cavitand-porphyrin complex)

RE.CNT 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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IT 172805-94-6P 172925-98-3P

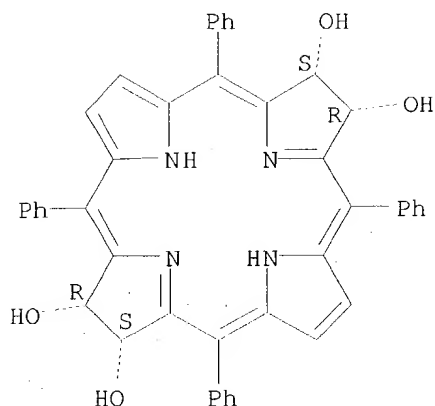
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation, oxidation to porphyrintetrone and subsequent reaction to give
zinc cavitand-porphyrin complex)

RN 172805-94-6 HCAPLUS

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-
tetraphenyl-, (7R,8S,17R,18S)-rel- (9CI) (CA INDEX NAME)

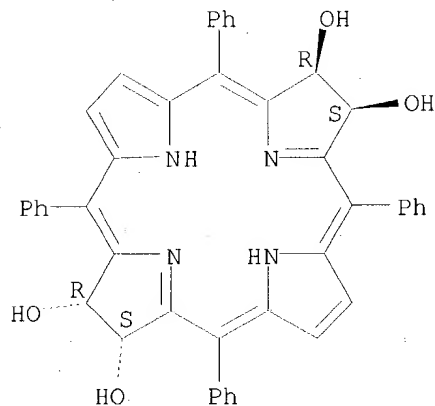
Relative stereochemistry.



RN 172925-98-3 HCAPLUS

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L55 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:831421 HCAPLUS

DN 134:100684

ED Entered STN: 29 Nov 2000

TI Functionalized diphenylchlorins and bacteriochlorins: their synthesis and bioconjugation for targeted photodynamic therapy and tumor cell imaging

AU Sutton, Jonathan M.; Fernandez, Nelson; Boyle, Ross W.

CS Department of Biological Sciences, University of Essex, Colchester, CO4 3SQ, UK

SO Journal of Porphyrins and Phthalocyanines (2000), 4(7), 655-658

CODEN: JPPHFZ; ISSN: 1088-4246

PB John Wiley & Sons Ltd.

DT Journal

LA English

CC 26-7 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 9, 22

OS CASREACT 134:100684

AB A range of 5,15-diphenylporphyrins with sym. and unsym. substitution patterns were subjected to osmium tetroxide-mediated dihydroxylations. The resulting chlorins and bacteriochlorins present an important group of compds. for studying structure-activity relationships of photodynamic

sensitizers. The regioselectivity of the dihydroxylation of various 5,15-diphenylporphyrins with unsym. substitution patterns was also examined Both diphenylchlorin diol (DPC) and diphenylbacteriochlorin tetrol (DPBC) examples were converted into reactive isothiocyanates and conjugated with bovine serum albumin (BSA).

- ST porphyrin diphenyl dihydroxylation regioselective; chlorin diphenyl dihydroxy tetrahydroxy prepn; diphenylchlorin bacteriochlorin isothiocyanate conjugate BSA
- IT Porphyrins
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (chlorins, di-Ph; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)
- IT Albumins, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (conjugates; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)
- IT Dihydroxylation
(stereoselective; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)
- IT Fluorescence
UV and visible spectra
(synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)
- IT 318488-18-5P 318488-24-3P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)
- IT 318488-06-1P 318488-12-9P 318488-23-2P 318488-29-8P 318488-30-1DP, conjugate with BSA 318488-31-2DP, conjugate with BSA
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)
- IT 22112-89-6, 5,15-Diphenylporphyrin 128374-05-0 253666-33-0
268737-71-9 318488-01-6 318488-02-7 318488-13-0 318488-14-1
318488-15-2 318488-16-3 318488-17-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)
- IT **165336-21-0P** 318488-03-8P 318488-04-9P 318488-05-0P
318488-07-2P 318488-08-3P 318488-10-7P 318488-11-8P 318488-19-6P
318488-20-9P 318488-21-0P 318488-22-1P 318488-25-4P 318488-26-5P
318488-27-6P 318488-28-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Adams, K; J Chem Soc, Perkin Trans 1 1992, P1465 HCAPLUS
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- (14) Hermanson, G; Bioconjugate Techniques 1978, P304
- (15) Jasat, A; Chem Rev 1997, V97, P2267 HCAPLUS
- (16) Kim, S; J Org Chem 1986, V3, P2613
- (17) Sternberg, E; Curr Med Chem 1996, V3, P239 HCAPLUS
- (18) Sternberg, E; Tetrahedron 1998, V54, P4151 HCAPLUS

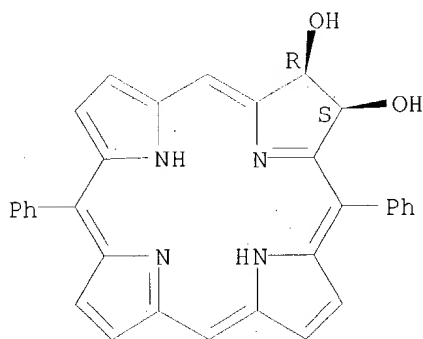
IT 165336-21-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

RN 165336-21-0 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-diphenyl-, (7R,8S)-rel- (9CI)
 (CA INDEX NAME)

Relative stereochemistry.



L55 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:742097 HCAPLUS

DN 133:296322

ED Entered STN: 20 Oct 2000

TI Synthesis of β, β , -dihydroxymeso
 -substituted chlorins, isobacteriochlorins, and
 bacteriochlorins with improved photosensitizer activity

IN Macalpine, Jill; Dolphin, David; Bruckner,
 Christian

PA University of British Columbia, Can.

SO PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D487-22

ICS A61K031-409; A61K049-00; A61P035-00; C07D487-22; C07D257-00;
 C07D209-00; C07D209-00; C07D209-00; C07D209-00

CC 26-7 (Biomolecules and Their Synthetic Analogs)

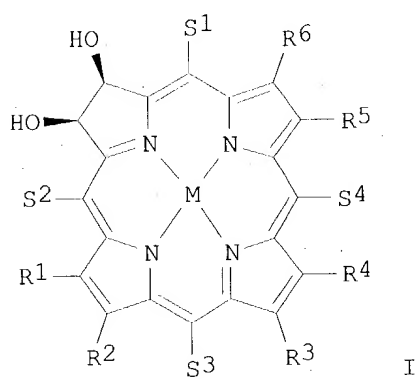
Section cross-reference(s): 1, 8

FAN.CNT 2

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WO 2000061584	A1	20001019	WO 2000-CA435	20000414
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,				

ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
 LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
 SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA,
 ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6620929 B1 20030916 US 2000-551160 20000414
 US 2004019201 A1 20040129 US 2003-622322 20030717
 PRAI US 1999-129324P P 19990414
 US 2000-551160 A1 20000414
 OS MARPAT 133:296322
 GI



AB Synthesis of β, β , -dihydroxymeso
 -substituted **chlorins** (I) [M = 2H, Ni(II), Cu(II), Zn, Sn, Ge,
 Si, Ga, Al, Mn(III), Gd(III), In, Tc; R1-R6 = independently H, alkyl,
 alkylcarboxylic acid or ester, =O, OH, NO₂, NH₂; taken together with
 another ring, ring substituent or meso substituent = fused 5- or
 6-membered ring; S1-S4 independently = H, (un)substituted alkyl,
 (un)substituted aryl, (un)substituted cycloalkyl, may be same or
 different], **bacteriochlorins**, and **isobacteriochlorins**
 with improved photosensitizer activity is described. Thus, I (S1-S4 = Ph,
 M = 2H, R1-R6 = H) (II) is prepared by treatment of tetraphenylporphyrin
 with osmium tetroxide. II shows an LD50 of 2.78 μ M in cytotoxicity
 assay.

ST arylchlorin dihydroxy prepn phototoxicity cytotoxicity;
 metallodihydroxyarylchlorins phototoxicity cytotoxicity; bacteriochlorin
 aryl tetrahydroxy prepn phototoxicity cytotoxicity; photosensitizer
 photodynamic therapy; tetraarylporphyrin stereoselective dihydroxylation
 osmium tetroxide

IT Porphyrins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or
 effector, except adverse); BSU (Biological study, unclassified); SPN
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
 PREP (Preparation); USES (Uses)

(**chlorins**, metallo-; synthesis of β ,
 β , -dihydroxymeso-substituted **chlorins**,
isobacteriochlorins, and **bacteriochlorins** with
 improved photosensitizer activity)

IT Dihydroxylation

(stereoselective, osmium tetroxide; synthesis of β ,
 β , -dihydroxymeso-substituted **chlorins**,
isobacteriochlorins, and **bacteriochlorins** with

improved photosensitizer activity)

IT Photodynamic therapy
Photosensitizers (pharmaceutical)
Phototoxicity
(synthesis of β , β , -dihydroxymeso
-substituted **chlorins**, **isobacteriochlorins**, and
bacteriochlorins with improved photosensitizer activity)

IT 51552-53-5P 165336-18-5P 165336-21-0P 172925-98-3P
301336-58-3P 301336-61-8P 301336-66-3P
301336-70-9P 301336-74-3P 301336-78-7P
301336-82-3P 301336-85-6P 301336-88-9P
301336-91-4P 301336-94-7P 301336-97-0P
301337-00-8P 301337-03-1P 301337-05-3P
301337-07-5P 301337-10-0P 301337-13-3P
301337-16-6P 301337-19-9P 301337-23-5P 301338-12-5P
301530-01-8P 301530-02-9P 301530-03-0P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or
effector, except adverse); BSU (Biological study, unclassified); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(synthesis of β , β , -dihydroxymeso
-substituted **chlorins**, **isobacteriochlorins**, and
bacteriochlorins with improved photosensitizer activity)

IT 7429-90-5P, Aluminum, preparation 7440-21-3P, Silicon, preparation
7440-26-8P, Technetium, preparation 7440-31-5P, Tin, preparation
7440-55-3P, Gallium, preparation 7440-56-4P, Germanium, preparation
7440-66-6P, Zinc, preparation 7440-74-6P, Indium, preparation
14546-48-6P, Manganese(III), preparation 14701-22-5P, Nickel(II),
preparation 15158-11-9P, Copper(II), preparation 22541-19-1P,
Gadolinium, ion(3+), preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of β , β , -dihydroxymeso
-substituted **chlorins**, **isobacteriochlorins**, and
bacteriochlorins with improved photosensitizer activity)

IT 74-88-4, Methyl iodide, reactions 917-23-7, Tetraphenylporphyrin
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of β , β , -dihydroxymeso
-substituted **chlorins**, **isobacteriochlorins**, and
bacteriochlorins with improved photosensitizer activity)

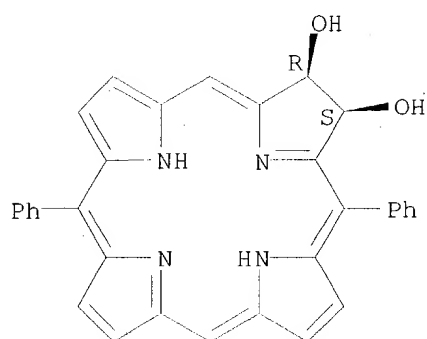
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Dolphin; US 5684485 A 1997
(2) Univ British Columbia; WO 9613504 A 1996 HCAPLUS

IT 165336-21-0P 172925-98-3P 301336-58-3P
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301336-74-3P 301336-78-7P 301336-82-3P
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301337-03-1P 301337-05-3P 301337-07-5P
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RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or
effector, except adverse); BSU (Biological study, unclassified); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(synthesis of β , β , -dihydroxymeso
-substituted **chlorins**, **isobacteriochlorins**, and
bacteriochlorins with improved photosensitizer activity)

RN 165336-21-0 HCAPLUS
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-diphenyl-, (7R,8S)-rel- (9CI)

(CA INDEX NAME)

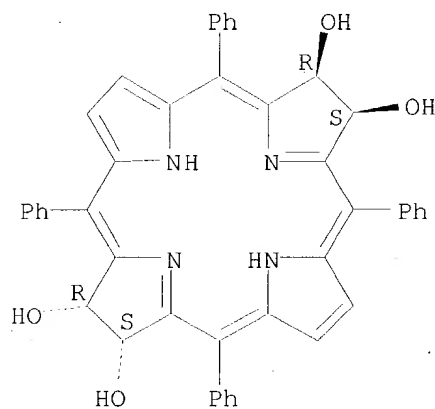
Relative stereochemistry.



RN 172925-98-3 HCAPLUS

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

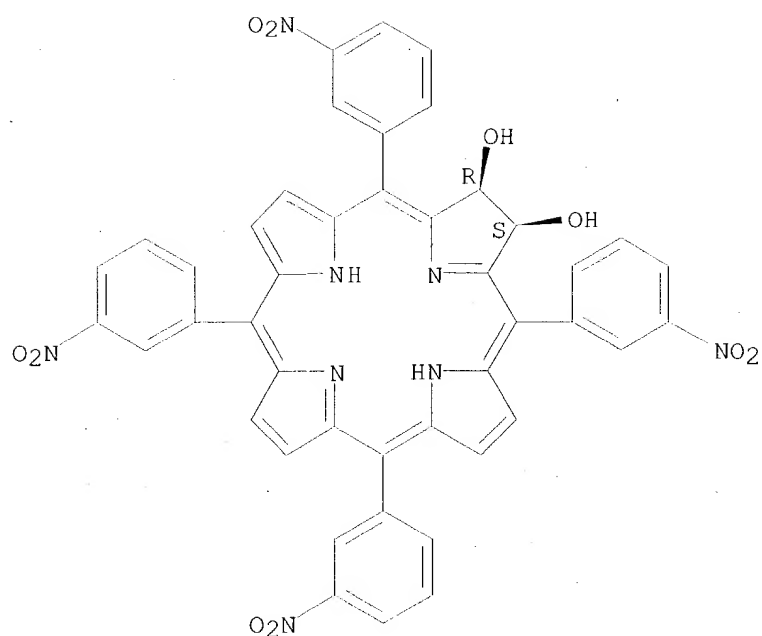
Relative stereochemistry.



RN 301336-58-3 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-nitrophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

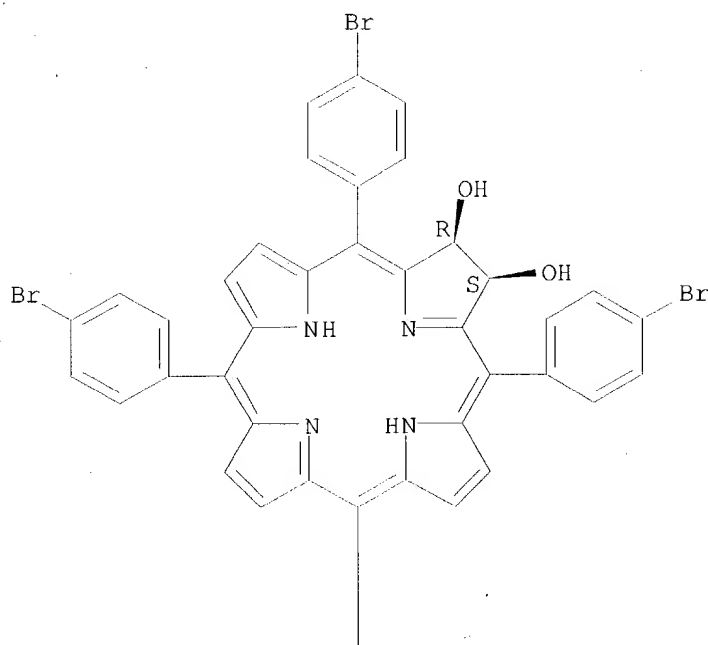


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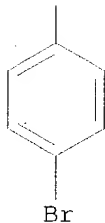
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(4-bromophenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

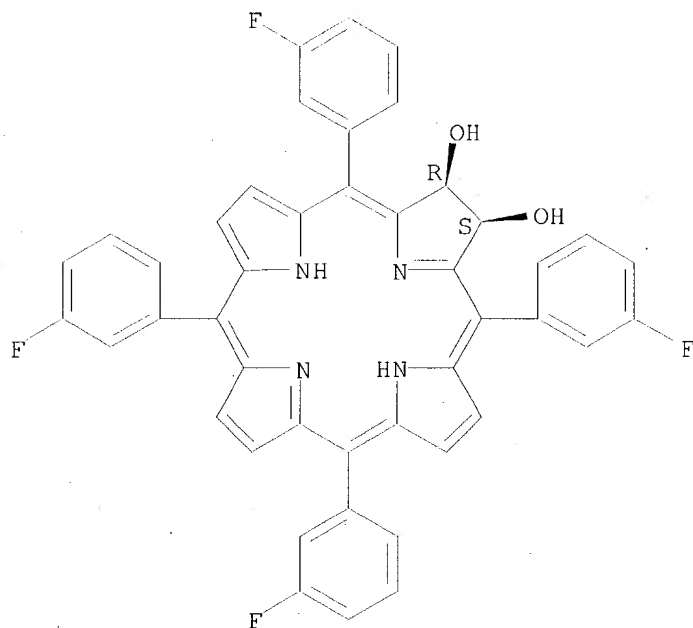


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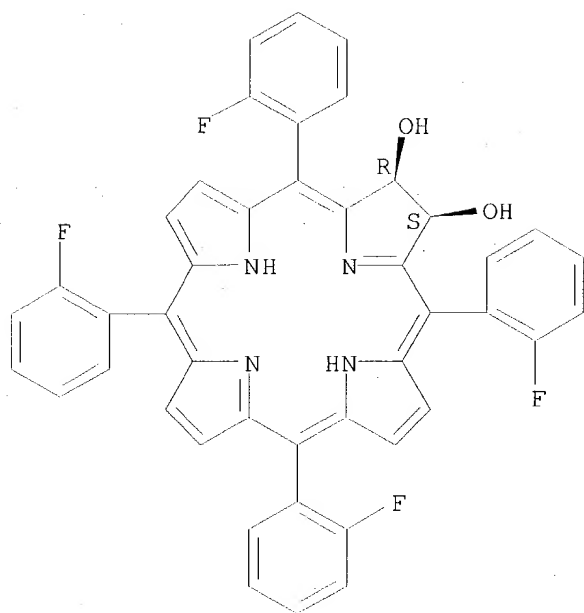
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CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3-fluorophenyl)-7,8-dihydro-
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 301336-70-9 HCAPLUS
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(2-fluorophenyl)-7,8-dihydro-
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

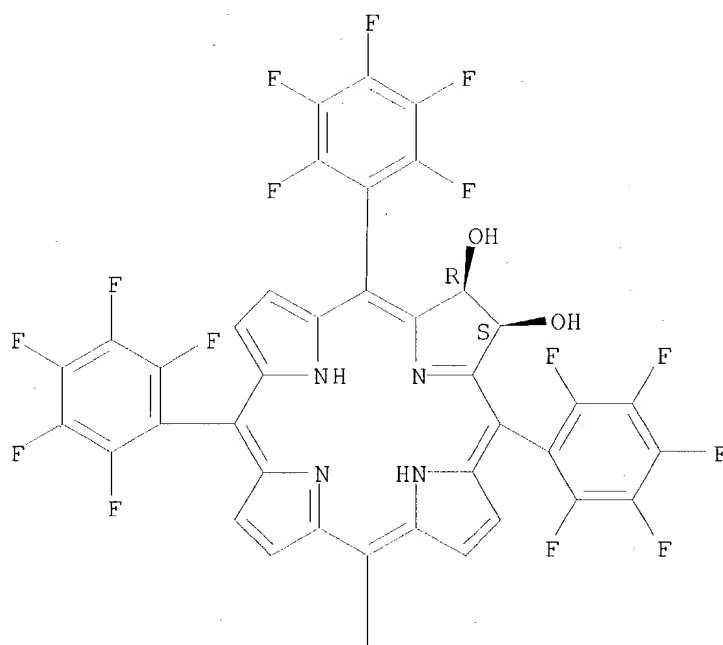
Relative stereochemistry.



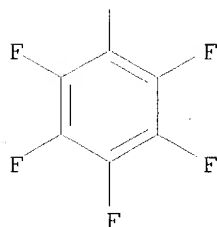
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CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(pentafluorophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

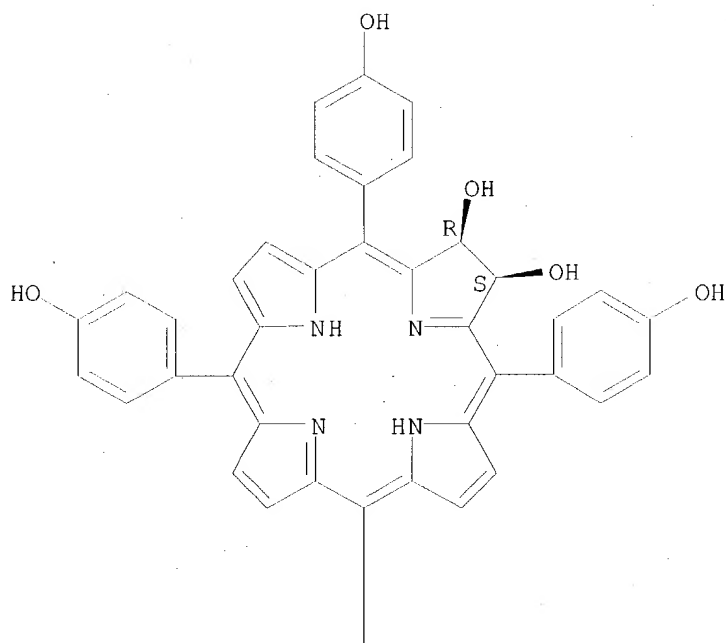


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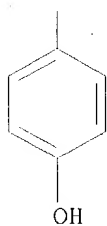
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



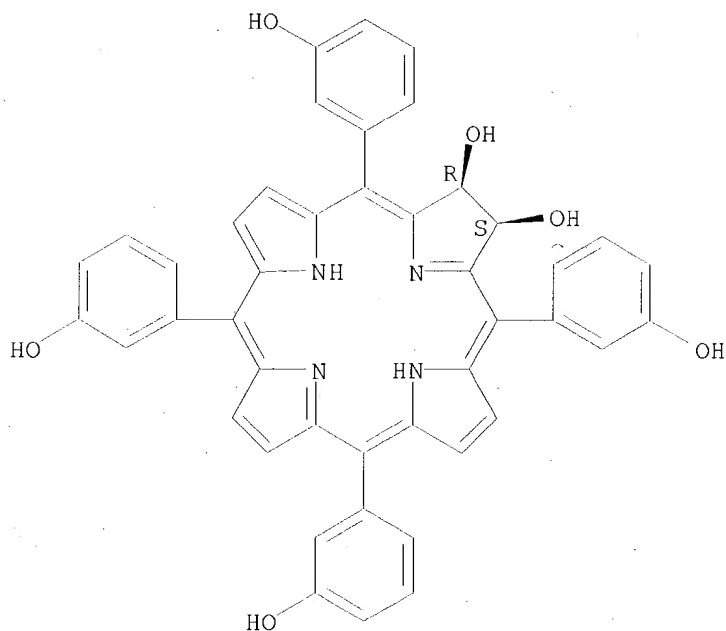
PAGE 2-A



RN 301336-82-3 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-hydroxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

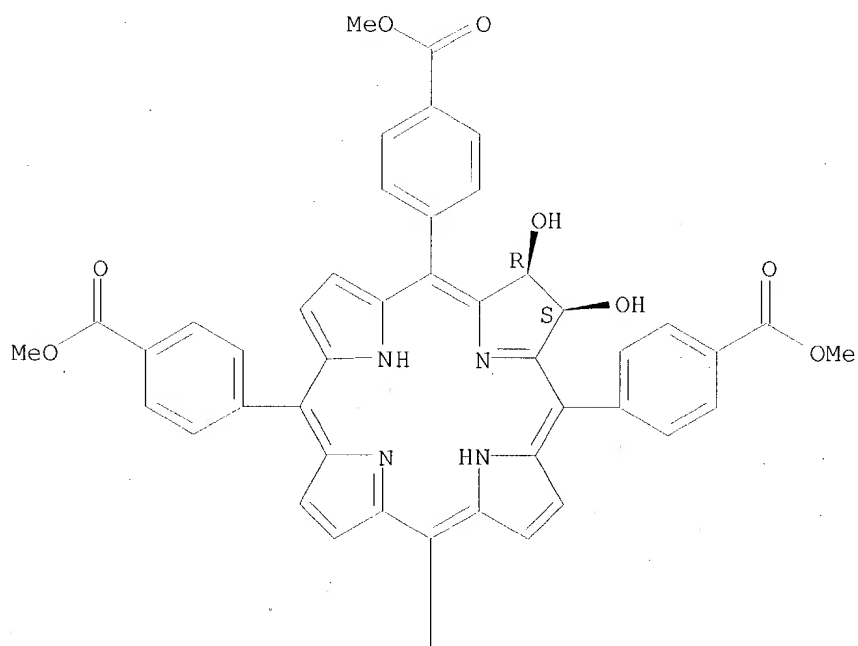


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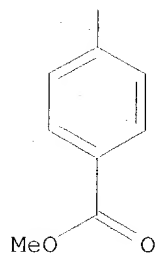
CN Benzoic acid, 4,4',4'',4'''-[(7R,8S)-7,8-dihydro-7,8-dihydroxy-21H,23H-porphine-5,10,15,20-tetrayl]tetrakis-, tetramethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

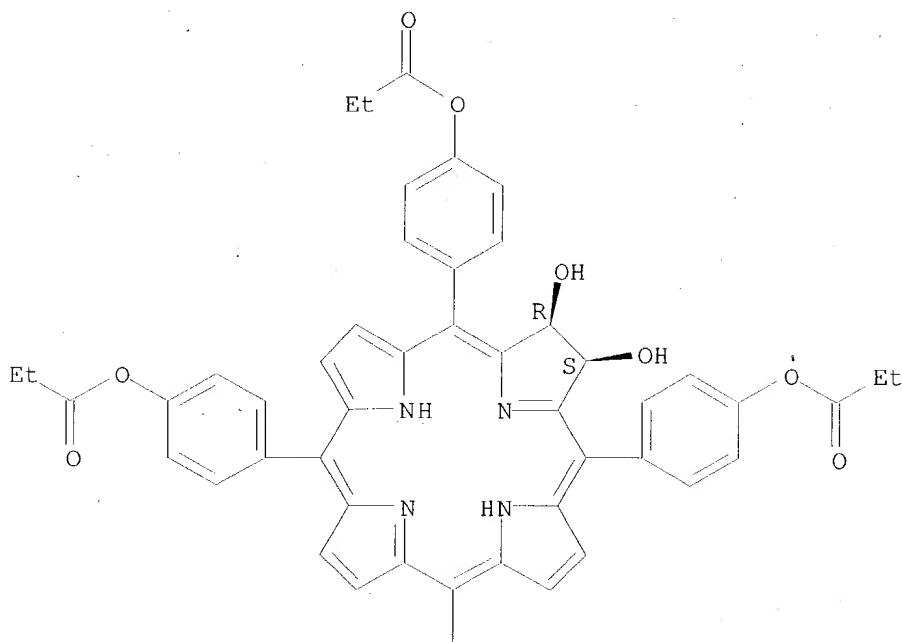


RN 301336-88-9 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis[4-(1-oxopropoxy)phenyl]-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

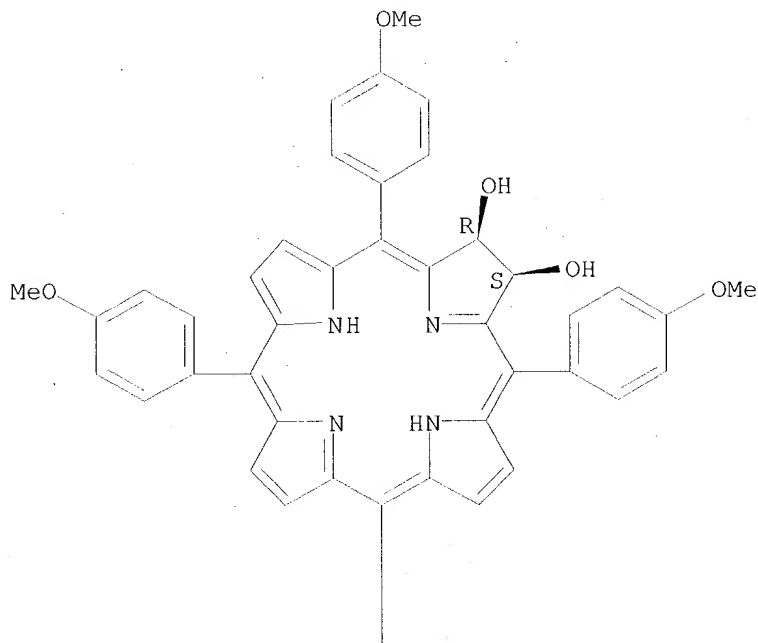
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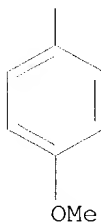
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CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

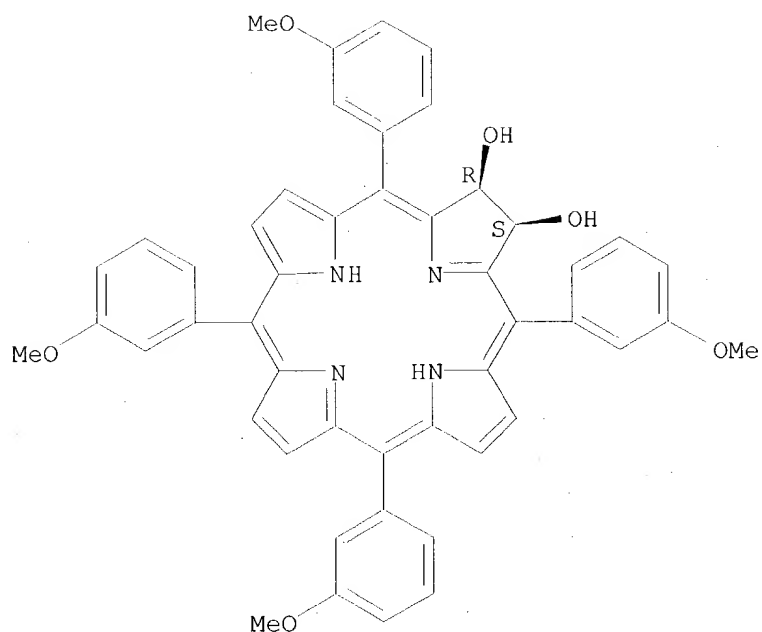


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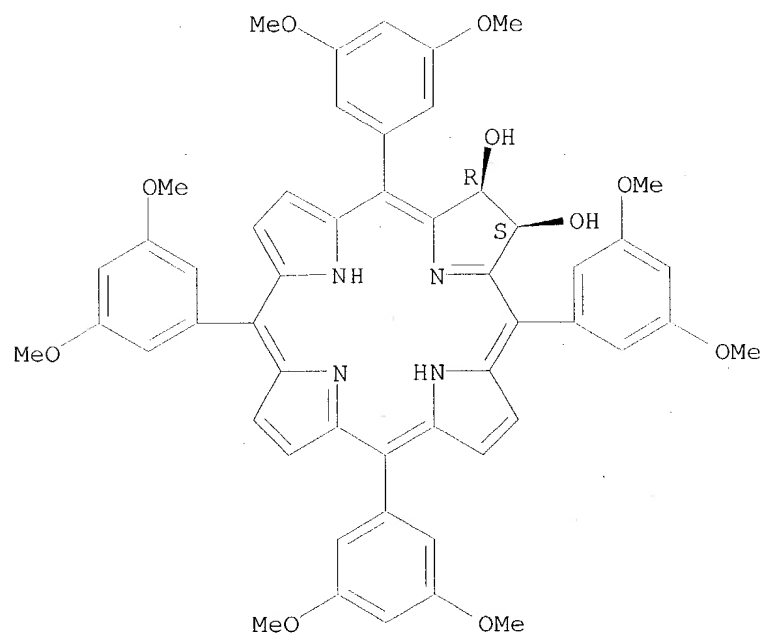
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CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 301336-97-0 HCAPLUS
 CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3,5-dimethoxyphenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

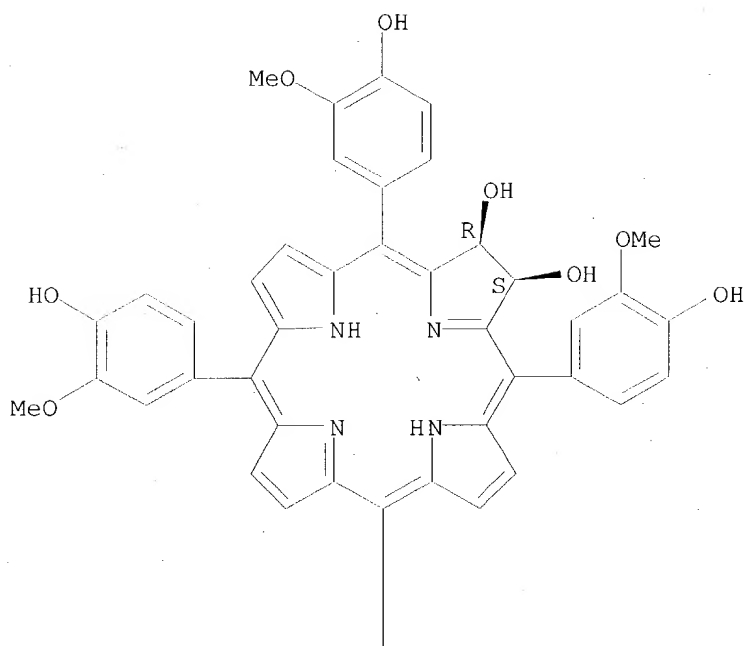
Relative stereochemistry.



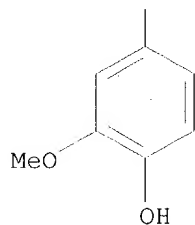
RN 301337-00-8 HCAPLUS
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxy-3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

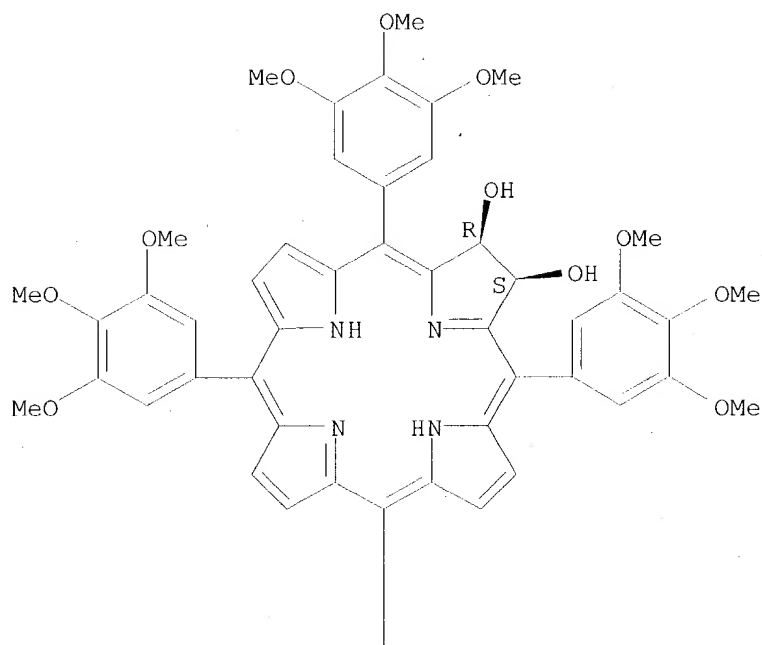


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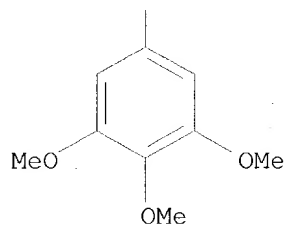
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3,4,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



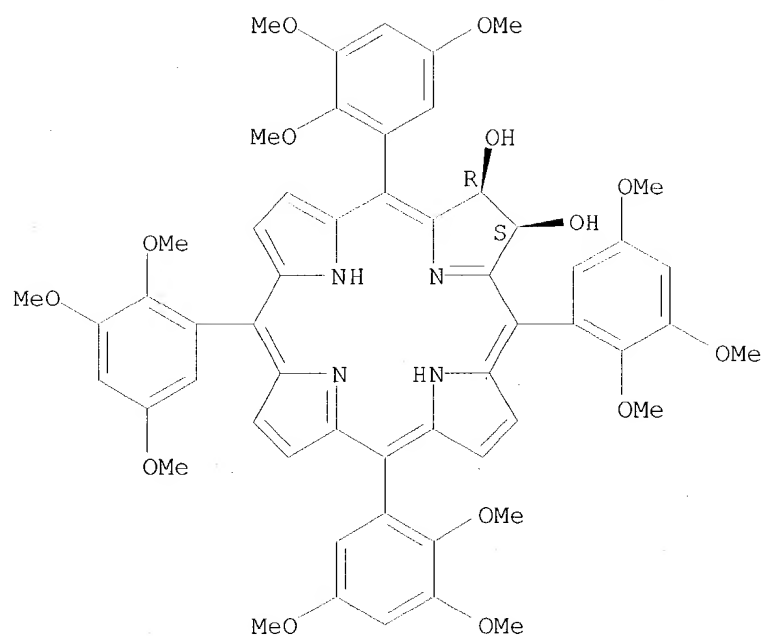
PAGE 2-A



RN 301337-05-3 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,3,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

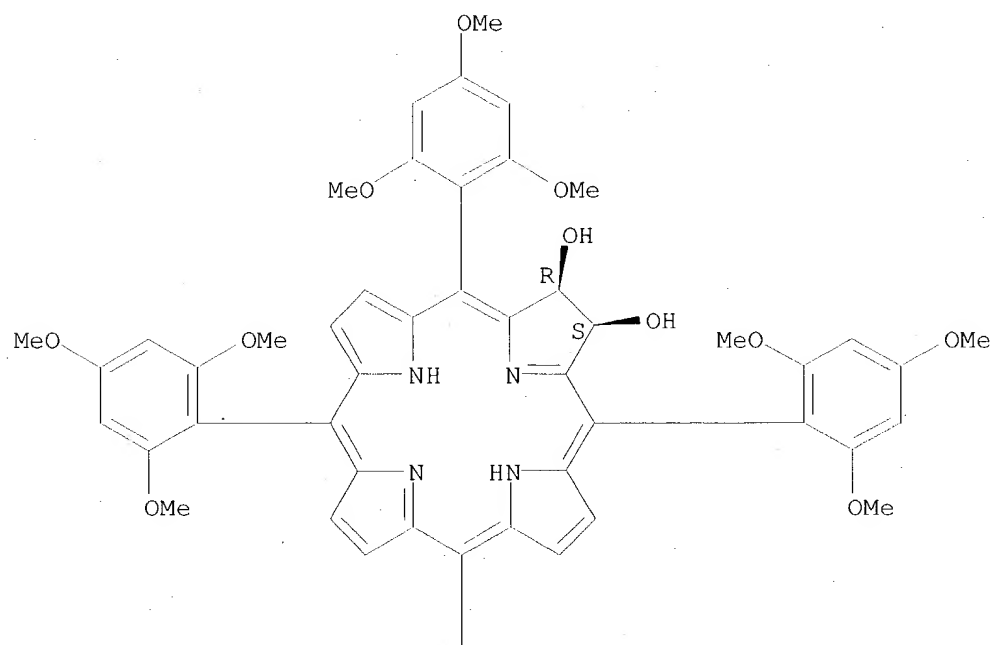


RN 301337-07-5 HCAPLUS

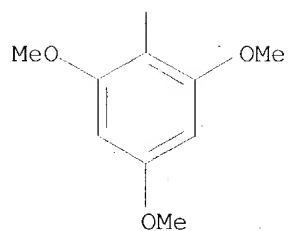
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,4,6-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

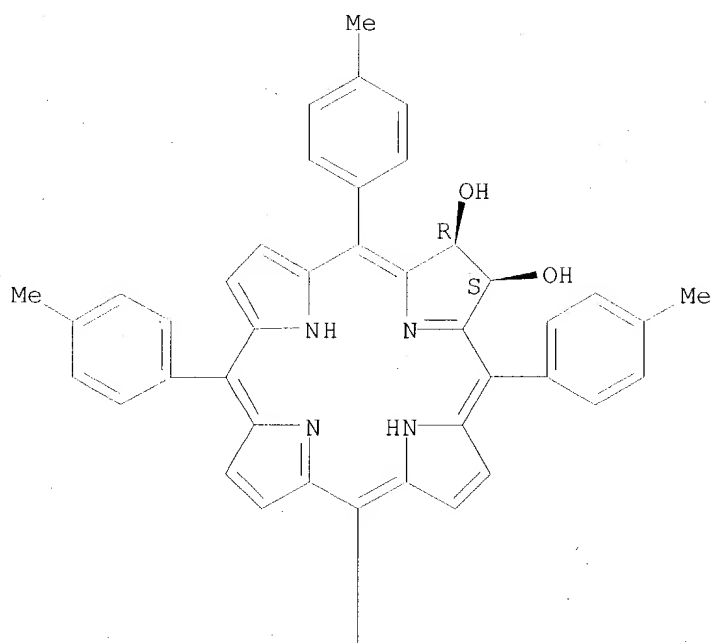


RN 301337-10-0 HCAPLUS

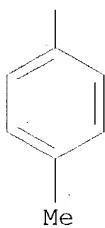
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methylphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

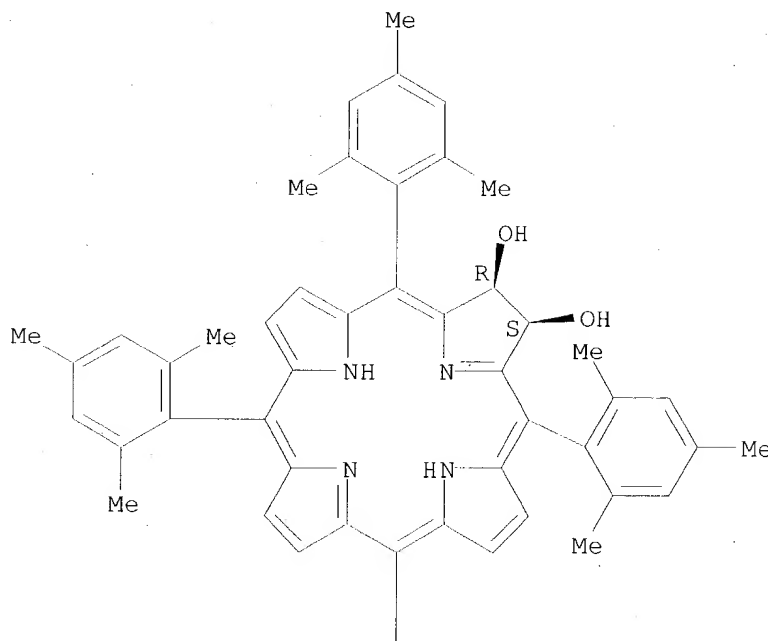


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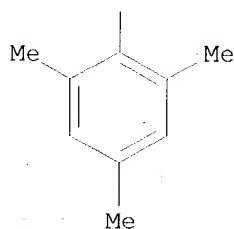
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

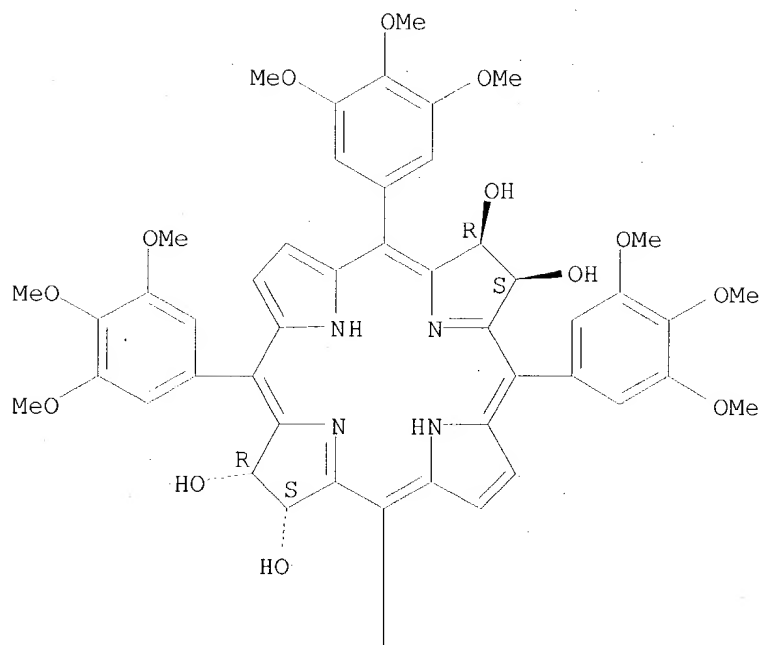


RN 301337-23-5 HCAPLUS

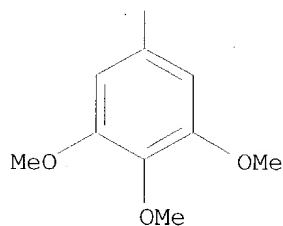
CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetrakis(3,4,5-trimethoxyphenyl)-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



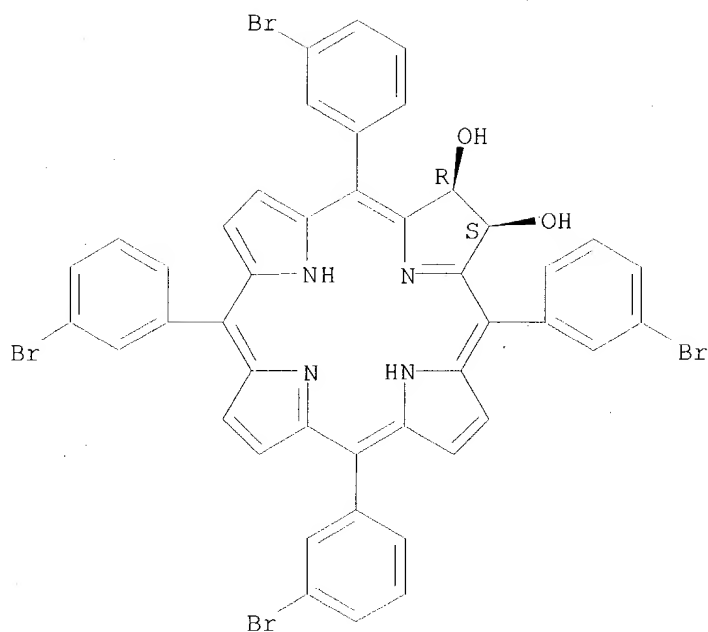
PAGE 2-A



RN 301338-12-5 HCAPLUS

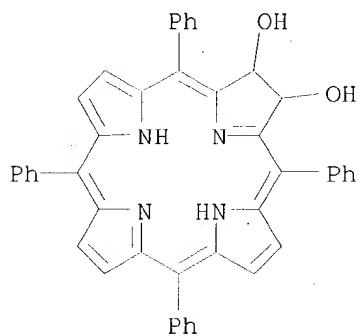
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(3-bromophenyl)-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 301530-01-8 HCAPLUS

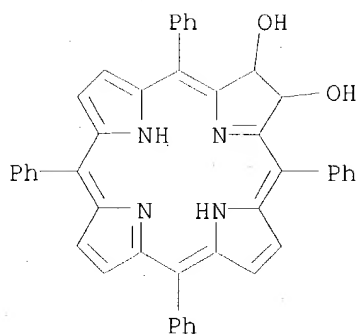
CN 21H,23H-Porphine-7,8-diol, 5(or 15)-(4-bromophenyl)-7,8-dihydro-
10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)



D1-Br

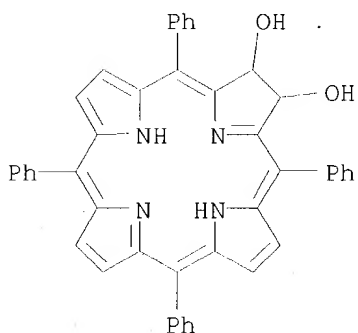
RN 301530-02-9 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5(or 15)-(4-hydroxyphenyl)-
10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)



D1-OH

RN 301530-03-0 HCAPLUS
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5(or 15)-(4-nitrophenyl)-
 10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)



D1-NO2

L55 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:391901 HCAPLUS
 DN 125:58205
 ED Entered STN: 09 Jul 1996
 TI β, β' -dihydroxy meso
 -substituted chlorins, isobacteriochlorins,
 bacteriochlorins
 IN Dolphin, David; Bruckner, Christian
 PA University of British Columbia, Can.
 SO PCT Int. Appl., 92 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07D487-22
 ICA A61K049-00; A61K031-40
 ICI C07D487-22, C07D257-00, C07D209-00
 CC 26-7 (Biomolecules and Their Synthetic Analogs)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9613504	A1	19960509	WO 1995-CA602	19951025

W: AT, AU, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KR, LU, MX,
NO, NZ, PL, PT, SE, SK

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

US 5648485	A	19970715	US 1994-329577	19941026
CA 2199399	AA	19960509	CA 1995-2199399	19951025
AU 9536951	A1	19960523	AU 1995-36951	19951025
AU 704971	B2	19990513		
CN 1161697	A	19971008	CN 1995-195859	19951025
CN 1043143	B	19990428		
EP 804439	A1	19971105	EP 1995-944791	19951025
EP 804439	B1	20030917		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE

HU 77008	A2	19980302	HU 1997-1702	19951025
JP 10507766	T2	19980728	JP 1995-514205	19951025
JP 2001294589	A2	20011023	JP 2001-94418	19951025
JP 3228296	B2	20011112	JP 1996-514205	19951025
PL 182239	B1	20011130	PL 1995-319907	19951025
AT 250064	E	20031015	AT 1995-944791	19951025
FI 9701734	A	19970423	FI 1997-1734	19970423
NO 9701952	A	19970425	NO 1997-1952	19970425
US 5831088	A	19981103	US 1997-853115	19970508

PRAI US 1994-329577 A 19941026
JP 1996-514205 A3 19951025
WO 1995-CA602 W 19951025

OS MARPAT 125:58205

AB Title compds. were prepared by osmylating a J,J'-unsubstituted, meso-substituted porphyrin to form an osmate ester at the β,β' -position and reducing the osmate ester to form the title compound. The compds. are useful in photodynamic therapy (no data). Thus meso-tetraphenylporphyrin was osmylated and reduced with H₂S to give the dihydroxy derivative in 49% yield.

ST osmylation tetraphenylporphyrin; porphyrin tetraphenyl osmylation; chlorin dihydroxytetraphenyl prepn photodynamic therapy; photodynamic therapy dihydroxytetraphenylchlorin prepn

IT Porphyrins

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dihydroxychlorins for use in photodynamic therapy)

IT Phototherapy

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(chemo-, preparation of dihydroxychlorins for use in photodynamic therapy)

IT 917-23-7, 5,10,15,20-Tetraphenylporphyrin 2669-65-0 14074-80-7
31183-11-6, Zinc, [5,10,15,20-tetra-4-pyridinyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-4-1)-

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dihydroxychlorins for use in photodynamic therapy)

IT 112374-51-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of dihydroxychlorins for use in photodynamic therapy)

IT 165336-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of dihydroxychlorins for use in photodynamic therapy)

IT 165336-19-6P 165336-20-9P 172805-91-3P **172805-94-6P**
172925-98-3P 178214-23-8P 178214-24-9P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dihydroxychlorins for use in photodynamic therapy)

IT **172805-94-6P 172925-98-3P**

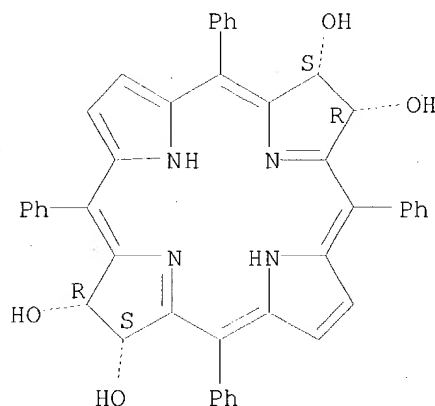
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

study); PREP (Preparation); USES (Uses)
 (preparation of dihydroxychlorins for use in photodynamic therapy)

RN 172805-94-6 HCAPLUS

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17R,18S)-rel- (9CI) (CA INDEX NAME)

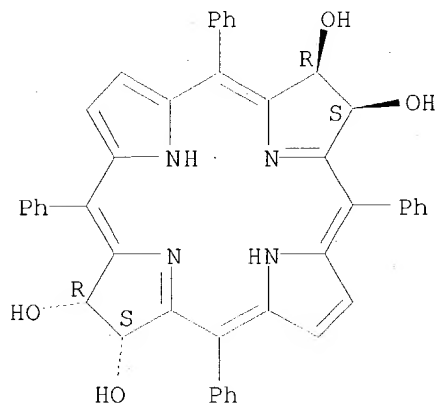
Relative stereochemistry.



RN 172925-98-3 HCAPLUS

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L55 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1996:14141 HCAPLUS

DN 124:116935

ED Entered STN: 06 Jan 1996

TI β,β' -Dihydroxylation of meso-tetraphenylchlorins and metallochlorins

AU Brueckner, Christian; Dolphin, David

CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Z1, Can.

SO Tetrahedron Letters (1995), 36(52), 9425-8

CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier

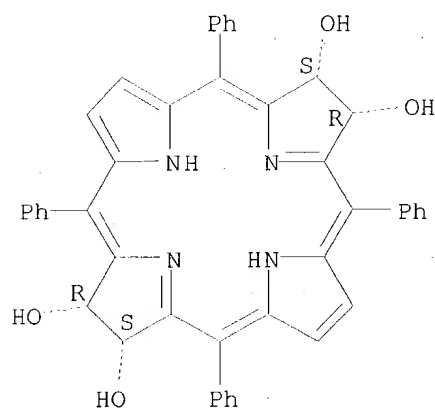
DT Journal

LA English

CC 26-7 (Biomolecules and Their Synthetic Analogs)

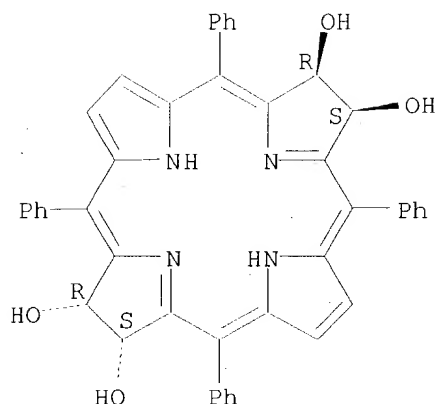
OS CASREACT 124:116935
 AB Meso-Tetraphenylchlorin and 2,3-vic-dihydroxy-meso-tetraphenylchlorin and their zinc complexes were dihydroxylated by stoichiometric amts. of OsO₄. The chlorins gave specifically 2,3-vic-dihydroxy-meso-tetraphenylbacteriochlorins or 2,3,12,13-bis-(vic-dihydroxy)bacteriochlorins while the Zn(II)-chlorins gave (2,3-vic-dihydroxy-meso-tetraphenylisobacteriochlorinato)Zn(II) or [2,3,7,8-bis-(vic-dihydroxy)-meso-tetraphenylisobacteriochlorinato]Zn(II).
 ST bacteriochlorin hydroxy prep; isobacteriochlorin hydroxy prep; dihydroxylation chlorin
 IT Phototherapy
 (chemo-, dihydroxylation of meso-tetraphenylchlorins and metallochlorins)
 IT Hydroxylation
 (osmylation, stereoselective, dihydroxylation of meso-tetraphenylchlorins and metallochlorins)
 IT 2669-65-0 14839-32-8 165336-18-5 165336-19-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (dihydroxylation of meso-tetraphenylchlorins and metallochlorins)
 IT 172805-92-4P 172925-99-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (dihydroxylation of meso-tetraphenylchlorins and metallochlorins)
 IT 172805-91-3P 172805-93-5P **172805-94-6P** 172805-95-7P
 172805-96-8P **172925-98-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (dihydroxylation of meso-tetraphenylchlorins and metallochlorins)
 IT **172805-94-6P 172925-98-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (dihydroxylation of meso-tetraphenylchlorins and metallochlorins)
 RN 172805-94-6 HCAPLUS
 CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17R,18S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 172925-98-3 HCAPLUS
 CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L55 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:567157 HCAPLUS
 DN 123:83046
 ED Entered STN: 23 May 1995
 TI 2,3-vic-Dihydroxy-meso-tetraphenylchlorins from the osmium tetroxide
 oxidation of meso-tetraphenylporphyrin
 AU Brueckner, Christian; **Dolphin, David**
 CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Z1, Can.
 SO Tetrahedron Letters (1995), 36(19), 3295-8
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier
 DT Journal
 LA English
 CC 26-7 (Biomolecules and Their Synthetic Analogs)
 OS CASREACT 123:83046
 AB Meso-tetraphenylporphyrins and meso-tetraphenylmetalloporphyrins were
 converted into stable 2,3-vic-dihydroxy-meso-tetraphenylchlorins and
 2,3-vic-dihydroxy-meso-tetraphenylmetallochlorins by oxidation with
 stoichiometric amts. of OsO₄ and subsequent reduction of the isolable osmate
 esters. The stable dihydroxychlorins were dehydrated under acid catalysis
 to yield 2-hydroxy-meso-tetraphenylporphyrins.
 ST osmylation tetraphenylporphyrin; tetraphenylchlorin dihydroxy prepn
 dehydration; chlorin dihydroxytetraphenyl prepn dehydration; porphyrin
 hydroxytetraphenyl
 IT Porphyrins
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (vic-dihydroxy-meso-tetraphenylchlorins by osmylation of
 meso-tetraphenylporphyrin)
 IT Porphyrins
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (chlorins, vic-dihydroxy-meso-tetraphenylchlorins by osmylation of
 meso-tetraphenylporphyrin)
 IT Hydroxylation
 (osmylation, vic-dihydroxy-meso-tetraphenylchlorins by osmylation of
 meso-tetraphenylporphyrin)
 IT 917-23-7, meso-Tetraphenylporphyrin 14074-80-7, Zinc
 meso-tetraphenylporphyrin 22112-89-6, 5,15-Diphenylporphyrin
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (vic-dihydroxy-meso-tetraphenylchlorins by osmylation of
 meso-tetraphenylporphyrin)
 IT 165336-16-3P 165336-17-4P 165336-18-5P 165336-19-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (vic-dihydroxy-meso-tetraphenylchlorins by osmylation of

L17 4 S L14 AND L16
L18 4 S L15,L17
L19 14 S L16 NOT L18
L20 2 S L19 AND NR>=1
L21 6 S L18,L20
L22 34 S L14 NOT L15-L21
L23 STR
L24 50 S L23
L25 31936 S L23 FUL
L26 STR L23
L27 50 S L26 SAM SUB=L25
L28 30770 S L26 FUL SUB=L25
L29 STR L26
L30 20493 S L29 FUL SUB=L28
L31 37 S L13 AND L25
L32 6 S L31 AND (BR OR F)/ELS
L33 5 S L32 NOT IDS/CI
L34 2 S L31 AND NITRO
L35 1 S L34 NOT IDS/CI
L36 1 S L31 AND METHYL ESTER
L37 0 S L31 AND ETHYL ESTER
L38 1 S L31 AND BENZOIC ACID
L39 8 S L31 AND METHOXY
L40 22 S L31 NOT L33,L35,L36,L38,L39
L41 7 S L40 AND (C44H34N4O4 OR C48H40N4O2 OR C44H32N4O6 OR C56H56N4O2
L42 22 S L33,L35,L36,L39,L41
L43 15 S L31 NOT L42
L44 16 S L13 NOT L31
L45 1 S L44 AND 46.150.18/RID
L46 23 S L42,L45
L47 15 S L14 NOT L46
L48 3 S L47 AND (C44H31BRN4O2 OR C44H31N5O4 OR C44H32N4O3)
L49 26 S L46,L48
SAV L49 FAY551/A

FILE 'HCAOLD' ENTERED AT 18:57:10 ON 12 FEB 2004

L50 0 S L49

FILE 'HCAPLUS' ENTERED AT 18:57:14 ON 12 FEB 2004

L51 9 S L49
L52 5 S L51 AND L1-L3
L53 5 S L12,L52
L54 4 S L51 NOT L53
L55 9 S L51-L54

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L56 3 S L49

FILE 'REGISTRY' ENTERED AT 18:58:04 ON 12 FEB 2004

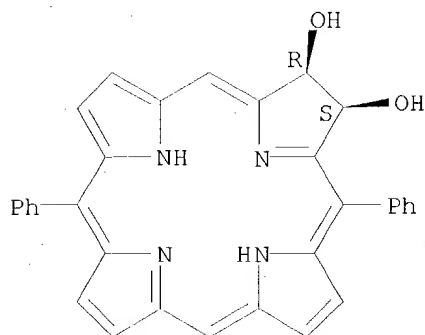
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FILE 'HCAPLUS' ENTERED AT 18:58:44 ON 12 FEB 2004

=>

meso-tetraphenylporphyrin)
 IT 102305-84-0P 165336-20-9P **165336-21-0P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (vic-dihydroxy-meso-tetraphenylchlorins by osmylation of
 meso-tetraphenylporphyrin)
 IT **165336-21-0P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (vic-dihydroxy-meso-tetraphenylchlorins by osmylation of
 meso-tetraphenylporphyrin)
 RN 165336-21-0 HCAPLUS
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-diphenyl-, (7R,8S)-rel- (9CI)
 (CA INDEX NAME)

Relative stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 18:03:21 ON 12 FEB 2004)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 18:03:37 ON 12 FEB 2004

E US2000-551159/AP, PRN
 E MACALPINE J/AU
 L1 6 S E5, E8-E10
 E MAC ALPINE J/AU
 E BRUCKNER C/AU
 L2 65 S E3, E4, E11
 E DOLPHIN D/AU
 L3 500 S E3-E6
 L4 4 S L1 AND L2, L3
 L5 13 S L2 AND L3
 L6 16 S L4, L5
 SEL DN AN 4
 L7 1 S E1-E3
 SEL DN AN L6 15
 L8 1 S E4-E6
 L9 2 S L7, L8
 L10 1 S BETA BETA DIHYDROXY MESO (L) ?CHLORIN?
 L11 1 S BETA BETA DIHYDROXYMESO (L) ?CHLORIN?
 L12 2 S L9-L11 AND L1-L11
 SEL RN

FILE 'REGISTRY' ENTERED AT 18:06:40 ON 12 FEB 2004

L13 53 S E7-E59
 L14 38 S L13 AND 46.150.18/RID
 L15 4 S L14 AND NR>=12
 L16 18 S L13 AND (NI OR CU OR ZN OR SN OR GE OR SI OR GA OR AL OR MN O